

NBS

TECHNICAL NOTE

448

STATUS REPORT

National Standard Reference
Data System

April 1968



U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards

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NBS

TECHNICAL NOTE 448

ISSUED JUNE 1968

STATUS REPORT

National Standard Reference Data System
April 1968

Edward L. Brady, Editor

Office of Standard Reference Data
Institute for Basic Standards
National Bureau of Standards
Washington, D.C. 20234

NBS Technical Notes are designed to supplement the Bureau's regular publications program. They provide a means for making available scientific data that are of transient or limited interest. Technical Notes may be listed or referred to in the open literature.

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STATUS REPORT

April 1, 1968

ABSTRACT

This report summarizes the status of activities of the NBS Office of Standard Reference Data as of April 1968. It provides a detailed review of the data compilation activities within the seven broad categories of the technical scope of the program: (1) nuclear data, (2) atomic and molecular data, (3) solid state data, (4) thermodynamic and transport data, (5) chemical kinetics, (6) colloid and surface properties, and (7) mechanical properties. Progress in data systems design and development and in information services are reviewed. Certain problem areas of the program are identified. The appendix includes: (1) a listing of information and data centers associated with the Office of Standard Reference Data, (2) publications of the National Standard Reference Data System, and (3) a listing of organizations, groups, or individuals compiling or evaluating data.

KEY WORDS

Nuclear data, atomic and molecular data, solid state data, thermodynamic and transport properties, chemical kinetics, colloid and surface properties, mechanical properties, data systems design and development, information services, standard reference data.

The report that follows has been written to give to the technical community of the United States an account of progress made by the NBS Office of Standard Reference Data in developing the National Standard Reference Data System. Since 1963, when the program came into existence, the magnitude of the effort required has been estimated more closely, procedures for the establishment of data centers have been developed, and relationships with other agencies have been more clearly defined. We have learned that the task of carrying out a critical evaluation is more demanding of both time and intellect than most members of the technical community undertaking these jobs had thought. The tasks involved have been clarified, and the qualifications of the staff needed within the data centers have been better formulated.

The original emphasis in the National Standard Reference Data System was on the production of compilations of critically evaluated data, with a somewhat lesser emphasis on the production of critical reviews. Operating experience has shown that, in addition, emphasis must be placed on critical analysis of the sources of uncertainty in the measurement results reported in the literature. Estimates made of the fraction of the literature in any specific field containing data worthy of a detailed critical evaluation range from approximately 50% down to a low of only 8 or 10%. Also, in almost every field in which a reasonably common measurement technique is employed, criteria need to be developed for the conditions under which experimental measurements should be made. Additional criteria should be agreed upon for the reporting of experimental results in the literature. Procedures are needed to ensure that results of quantitative measurements are made available to the data analysis center, even though they may not be reported in formal archival literature. In each of the fields in which the NBS Office of Standard Reference Data is active, these needs are to be examined in detail.

Progress in the NSRDS has been slower than desirable; initial plans four years ago called for much more rapid development. The rate of development has, of course, been determined by the availability of financial resources, which have been only a relatively small fraction of those estimated to be required to accomplish expeditiously the desired task. Nevertheless, many useful products have appeared. At the time of writing this report, 31 separate compilations and 6 critical reviews have been published or are in press; 16 non-critical compilations or bibliographies have appeared. Others are working their way through the pipeline to the point of public appearance.

As these products appear, greater attention is being paid to the general problem of making them most readily accessible to the technical community. In business terms, this is a marketing problem. We have asked the question, 'How should we market our products and services in

order to accomplish the most good for the progress of science and technology in the United States?" We are confident that a variety of marketing procedures must be employed, and we are gathering the information needed to develop plans for operation.

This report is presented to the technical community as an account of our custodianship of the NSRDS. We want to let you know what we are doing. We hope that you will let us know what you like and what you don't like. We welcome suggestions, comments, and criticisms from anyone who can help us achieve our goals.

April 1, 1968

Edward L. Brady

STATUS REPORT

THE NATIONAL STANDARD REFERENCE DATA SYSTEM

April 1, 1968

I. GENERAL SURVEY

A. Origin of National Standard Reference Data System

In June 1963, the Director of the President's Office of Science and Technology and the Federal Council for Science and Technology promulgated a Federal Policy establishing the National Standard Reference Data System. The NSRDS is envisioned as the total federal effort leading to the systematic production of compilations of critically evaluated quantitative data on the physical and chemical properties of substances and materials. According to the statement of the Director of OST, "The intent is to provide an articulated system of activities under such coordination and direction as to ensure a compilation of data meeting quality standards, and also to maintain continuous policy guidance of the system at the level of the Executive Office." Prior to the establishment of the NSRDS, many government agencies had been sponsoring activities of the type encompassed within the new system but without central coordination or policy guidance. To avoid duplication and at the same time to assure adequate and timely technical coverage, the Federal Council for Science and Technology decided that additional measures needed to be taken. The National Standard Reference Data System was the result.

In view of the statutory responsibilities of the National Bureau of Standards for measurement science and technology and for distribution of the results of measurements, NBS was considered to be the appropriate government organization to administer the NSRDS. The directive establishing the system calls upon the NBS to promote the basic objective of providing standard reference data to the technical community of the United States, to coordinate standard reference data activities of DoD, AEC, NASA, NSF, Commerce, Interior, and other government agencies; to operate a national standard reference data center at NBS; to establish standards of quality for various products of the NSRDS; and to establish standards of methodology and such other functions as are required to ensure the compatibility of all units of the NSRDS.

B. NBS Office of Standard Reference Data

In order to fulfill his responsibilities to the National Standard Reference Data System, the Director of the National Bureau of Standards has established the Office of Standard Reference Data within the NBS Institute for Basic Standards. The Office of Standard Reference Data has been assigned coordination and contracting responsibility for the

conduct of the NBS role in the NSRDS. It has monitoring responsibility but not direct operational responsibility for the data centers within and outside NBS that constitute the NSRDS. The present report contains a brief review of the actions taken and progress made by the Office of Standard Reference Data since its establishment, together with brief descriptions of the important systematic, continuing data compilation projects considered to comprise the major part of the National Standard Reference Data System.

C. Plan of Operation

The basic philosophy behind the plan of operation of the National Standard Reference Data System is that the program is a cooperative endeavor of the entire technical community of the United States. Its premise is that preparation of compilations of critically evaluated property data is of vital interest to nearly every technical man in the practice of his profession, and the needs and wishes of these men are to be determining factors in the guidance of the system. Most technical agencies of the government have found it necessary to sponsor data compilation activities of the type appropriate to the NSRDS in order to fulfill the requirements of their missions; these activities, by virtue of their very existence, are part of the total complex making up the National Standard Reference Data System.

In this system, though the National Bureau of Standards has assumed a special role — in accordance with the directive from the Office of Science and Technology — the NBS makes no proprietary claims to ownership of the NSRDS and endeavors at all times to maintain two-way channels of communication with persons involved with the development of the program in all agencies, both governmental and nongovernmental.

As stipulated in the OST-FCST Directive, the technical scope of the National Standard Reference Data System is physical science. For management purposes within the NBS Office of Standard Reference Data, the scope has been divided into seven broad categories: (1) nuclear data, (2) atomic and molecular data, (3) solid state data, (4) thermodynamics and transport data, (5) chemical kinetics, (6) colloid and surface properties, and (7) mechanical properties. In each of these categories an effort has been made to identify properties of interest, survey existing activities, establish priorities for expansion of existing projects and for initiation of new ones, and to enter into contractual or other financial arrangements with individuals or groups who are both competent and interested in doing the required work.

In all of these tasks, the NBS Office of Standard Reference Data has relied heavily upon consultation with panels of specialists in the fields of data. These panels of specialists are convened as subpanels of a general Advisory Committee under the auspices of the National Academy of Sciences-National Academy of Engineering. This committee is chaired by Frederick D. Rossini, Vice President for Research, Notre Dame University, whose personal knowledge, energy, and determination have

contributed much to the development of the program. The NAS-NAE Office of Critical Tables has served as organizer and secretariat for the panels of specialists and has greatly assisted the NBS Office of Standard Reference Data in communicating with the technical community of the United States. Further, the Office of Critical Tables has functioned as a primary channel of communication with related activities in other countries, especially those stimulated by the Committee on Data for Science and Technology (CODATA) of the International Council of Scientific Unions.

Some of the projects sponsored by the NBS Office of Standard Reference Data are conducted within the experimental divisions of the NBS. Others are in university laboratories; a few are in private industrial organizations. Some projects are funded solely by NBS; others jointly with other Federal agencies. A few are funded by other agencies with monitor responsibility delegated to NBS. A number of projects funded by other agencies are considered to be part of NSRDS because the output is of appropriate nature.

D. Operational Criteria for Projects

The level of effort in each project supported by the Office of Standard Reference Data is determined by a practical compromise involving three considerations: (1) the degree of comprehensiveness of the literature review, (2) the procedure for critical evaluation applied to the data, and (3) the need for continuity in updating the compilations. These three considerations require further discussion.

(1) Comprehensiveness — The raw material for any data compilation project is the result of measurements made by scientists in any part of the world. Normally, these results are reported in the literature, but sometimes in journals which may be obscure or difficult to obtain. Moreover, an increasing fraction of results worth saving for posterity is now appearing in government reports. Furthermore, in some areas (one example is data on neutron cross sections) many of the data generated in the laboratory never appear in any report or publication; in such instances the compiler personally may have to pry the data from the measurer. For a specific case, the degree of comprehensiveness that can be achieved must be a practical compromise between the desired 100% and the cost in time, money, and effort of achieving that goal. For most existing projects the comprehensiveness probably attains 90 to 99.8%.

(2) Critical evaluation — The procedure for "critical evaluation" varies widely from project to project. In present practice in some data centers, the experimental technique is reviewed, calculations are spot-checked, values of the fundamental constants are checked to ensure that the latest values were used, the temperature scale and other bases of measurement are checked (if appropriate), and limits of experimental uncertainty are independently assessed. In other centers, the data evaluator may decide, for intangible reasons that he may find difficult to formulate, that one particular value in the literature is "better" than another value. Such a judgment by a specialist of broad experience should

not be underrated; the value obtained is more likely to be accurate than the result of unweighted averaging. Most people agree that the first procedure provides a better "critical evaluation" than the second. However, for the practical purposes to which many compilations are applied, such a review is not justified, and the second procedure, or an intermediate one, is employed. The question immediately arises, then, of what degree of critical evaluation is required for a compilation to be considered "standard" reference data. It is probably desirable to use the word "standard" sparingly; it has connotations that apply to few existing compilations. For the present, when measurement results for most properties are uncertain and many are in dispute, the shorter term "reference data" would avoid the implications aroused by use of the word standard.

This matter has been discussed with the NAS-NAE Advisory Committee for the Office of Standard Reference Data, and the Committee has recommended that the two terms "standard reference data" and "reference data" be carefully distinguished and carefully used. This question is of such importance for the operations of the Office of Standard Reference Data that the relevant portion of the Advisory Committee report is given below:

It is now clear that the names "National Standard Reference Data System" and "National Standard Reference Data Program" contain a problem. The difficulty is the word "standard." By itself, the word "standard" may convey to the user a sense of authority which may be inappropriate for a given tabulation of data. Further, the National Bureau of Standards becomes involved in what may be a misleading way when a product of one of its programs carries the designation "standard." Thus, it is important to define what is meant by the terms "standard" data and "reference" data.

We can categorize "standard" data as those numerical values that serve as necessary tie-points in describing the physical universe for the scientific and technical community. Such "standard" values would be used by all compilers and experimenters in all countries. Some examples of "standard" data are:

- I. (1) The fundamental units of measurement — length, mass, time.
- (2) The recommended values of the fundamental physical constants as agreed on by international consensus, including the experimentally evaluated basic values, the defined values, and the derived values.
- (3) Fixed points on the International Temperature Scale, including the defining temperature of 273.16 K for the triple point of water.
- (4) The international scale of atomic masses.

II. (1) Anchor points in the structure of thermochemical, thermodynamic, and other tables, such as the heats of formation under standard conditions at 25 °C for water, carbon dioxide, hydrochloric acid, sulfuric acid, etc.

(2) Specific property values for chemical substances of certified high purity issued as standards by national standardizing laboratories for purposes of calibration of instruments or for intercomparison of the results of measurements made in different laboratories.

(3) Values of specified properties, determined in accordance with procedures and controls developed by committees of international experts, e.g., Class I Spectra (infrared) as defined by the Coblenz Society.

"Standard" values must always be accompanied by a numerical value of an assigned uncertainty. Defined values are numerically exact, that is, the uncertainty is zero. In many cases their use will be recommended by a national or international scientific body.

The Committee recommends use of the term "reference data" for numerical property values which originate through appraisal of the best available experimental data by competent experts who select best values, but which do not qualify as "standard" values as defined in the previous paragraph.

"Standard reference data," the ultimate goal of NSRDS, are to be striven for constantly, but perhaps not reached in many fields for years. Because of the variation in procedures for critical evaluation, it is intended that all future publications of NSRDS contain a statement of the criteria used for judgment and the argumentation used to derive the recommended values. Some compilations will be labeled "standard reference data"; some will be labeled "reference data." The criteria for decision have yet to be formulated.

(3) Continuity — For each individual compilation project, requirements for continuity must be examined. The overall program of NSRDS is designed to ensure continuity of effort in production of data compilations needed by scientists and engineers. In some areas a revised and updated compilation may be needed every 6 months; in others, only every 4 or 5 years. In almost all areas, continuing literature review and indexing operations are required to maintain a current awareness of the state of development of the field. Therefore most new projects undertaken by NSRDS are expected to be long-term, continuing activities, maintained as one component of the normal range of professional activity of the leader of the program.

E. Products of Data Centers

The original intent of the Office of Standard Reference Data was to stimulate the production of critically evaluated data compilations and critical reviews only and to give very little attention to bibliographies or other possible documentation aids to individuals. Experience in the operation of data centers has shown that only a slight additional effort is required in many cases to obtain some of these other products and that the user community finds them useful.

An examination of the sequence of events in a data center clearly shows why these other products are so readily obtained. Figure 1 is a schematic diagram of the broad types of activities and products that are normally associated with a data center. The left-hand column represents activities, while the right-hand column indicates a product that may result from the corresponding activity on the left. Following the initial selection of relevant papers from the literature (an activity basic to

INFORMATION ANALYSIS CENTERS

ACTIVITIES AND PRODUCTS

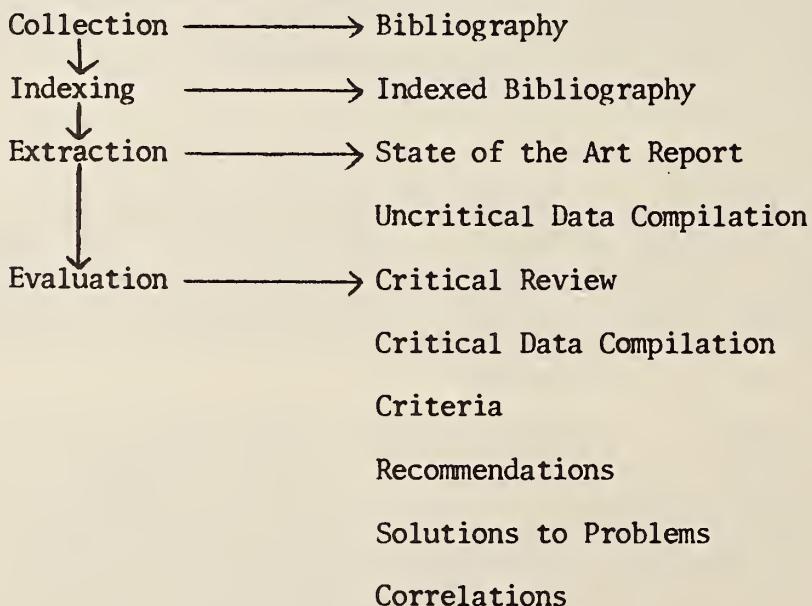


FIGURE 1. Activities and products of data evaluation centers.

all evaluation and compilation projects), a bibliography may be prepared, in which the literature to be evaluated is classified into several relatively broad categories. After the initial selection, the papers are indexed; this process consists of assigning a number of key words or symbols to each paper to indicate the data content of the reference. The indexed bibliography resulting from this activity is very useful to many groups of specialists. Indeed, some of the members of our advisory panels have stated they need nothing more; they would prefer to evaluate the data themselves. This, however, is the view of specialists in the field; a non-specialist who seeks a number to insert into a calculation prefers that an expert do the evaluation.

Figure 2 shows a page from one of the most comprehensive and successful of these indexed bibliographies, called CINDA (Computer Index to Neutron Data); it is concerned with sources of data on neutron cross sections. The first several columns contain symbols and numbers representing the target nucleus, the range of incident neutron energy, identification of the reference in a list following the table, and identification of the laboratory at which the measurements were carried out. Next come additional remarks characterizing the measurement more fully, the date of addition of the item to the computer file, identification of the person who prepared the entry, and an accession number for the entry. CINDA is particularly noteworthy because it represents the combined efforts of scientists in the United States, the United Kingdom, France, Germany, the U.S.S.R., and other countries. (The U.S. Atomic Energy Commission has sponsored the U.S. effort on CINDA; the NBS Office of Standard Reference Data has had no participation in this project.)

The next step in the production of a critical compilation is the extraction of data from the relevant literature. At this stage an uncritical compilation could be issued, if such is determined to be useful to the technical community. Figure 3 is an example of this kind of product; it shows a print-out of data on the ionization and appearance potential of cyanogen ion, retrieved from the files of the Mass Spectrometric Data Center at the National Bureau of Standards in Washington. This material is printed out as required to satisfy the requests of individual inquirers.

The preliminary activities of literature selection, indexing, and extraction of data lead finally to a critical evaluation of the data. The product of this work is a critical review of the state of quantitative knowledge in some limited area of a field, or a compilation of critically evaluated data. For NSRDS, a published product must contain sufficient argumentation for the user of the data to know how the results were obtained, as well as appropriate reference to the sources of the data used in the final evaluation. Figure 4 shows a page from a typical product of this type, with data expressed in the form of a table of numbers; data might also be expressed graphically.

Because bibliographies and uncritical data extractions are relatively easy to prepare once the basic work has been done, centers associated with NBS have been encouraged to prepare them if a user group wants them. Examination of the list of publications in this status report will show a significant number of such publications.

ELEMENT S Z A	QUANTITY	ENERGY MIN MAX	REFERENCE DATE	TYPE	LAB	REMARKS OR VALUES	MAY	1	1965	PAGE	257	CHRONUM
							NO.					
CR 24 050	N, N PROTON	14 7	NP 63 615	3/65	THEO-JOUR GER	BUTTNER+ STAT MOL CALC CFD XPT	650420EU	500866				
CR 24 050	N, N PROTON	14 7 16 7	NP 63 615	3/65	THEO-JOUR GER	BUTTNER+ STAT MOL CALC WITH G COMP	650420EU	500867				
CR 24 050	ENERGY LVLS		PRL 1 307A	0/58	-	PORTERBARTOL 780KV AS XPECTOFOR2P	650210U	9225				
CR 24 050	ENERGY LVLS		BAPS112 468	0/58	-	PORTERBARTOL 780KV PPPR 2P NEW LVL	650210U	9226				
CR 24 050	ENERGY LVLS		PR 112 468	0/58	-	INELAS SCAT P(R) OBS	650210U	9227				
CR 24 051	RESON PARAMS		PR 109 1243	2/58	-	JNSON ORNL INV PN OFFPHOLS PSTRFN	650210U	584				
CR 24 051	SPECT NGAMMA	THR	PR 125 2037	3/62	-	COIN CS GAM ENERGY LVL SCHEME	650210UA	585				
CR 24 051	N, ALPHA	14 7	NP 60 49	N/64	THEO-JOUR USA	GARDNER PREDICTED BY EMPIRICAL FORM	650407EU	500868	SAC			
CR 24 052	TOTAL XSECT	40 3 30 5	*PG NEWSON	6/56	-	OUKE	650210U	586				
CR 24 052	TOTAL XSECT	KEV	PR 111 288ANL	7/58	-	COTE TRNS ONLY NO RES BELO 15KEV	650210U	587				
CR 24 052	TOTAL XSECT	85 4 65 5	AP 17 319DUKE	3/62	-	650210UC	588					
CR 24 052	TOTAL XSECT	1 4 65 5	BAPS7 289G11	4/62	-	OUKE NOG RES PAR	650210UK	589				
CR 24 052	TOTAL XSECT	98 5	NP 54 417	6/64	THEO-JOUR OXF	OPTMOL FIT TO TOME GILBOY	650210UU	18655				
CR 24 052	RESON PARAMS	51 4 14 5	*PG NEWSON	6/56	-	OUKE CHIEFLY WT 4RES	650210U	590				
CR 24 052	RESON PARAMS	51 4	ANL 5498 P60	6/56	-	B9B ON W 28 2 538 S 1D2 1D7KEV	650210U	591				
CR 24 052	RESON PARAMS	40 5 41 5	ANL 5554H180CN	8/56	-	WT A ASS 30 LVL5	650210U	592				
CR 24 052	RESON PARAMS	51 4 41 5	PR 108 414ANL	0/57	-	H180DN 11E05 WN	AIRSLN	593				
CR 24 052	RESON PARAMS	KEV	PR 111 288ANL	7/58	-	COTE TRNS ONLY NO RES BELO 15K5V	650210U	594				
CR 24 052	RESON PARAMS	51 4 65 5	AP 17 319DUKE	3/62	-	S AND NON-S-RES PAR.NUC.TEMP=1.20	650210UC	595				
CR 24 052	RESON PARAMS	RES	NSA 16 3245	9/62	-	ABSTR 24818, OUKE THESIS, NOG	650210UT	596				
CR 24 052	STRNTH FNCTN	40 5 41 5	ANL 5554H180BN	8/56	-	2P2 AVGOF10RES SMALL GB TH CR53	650210U	597				

FIGURE 2. Illustrative page from CINDA, an indexed bibliography (Reference 1).

Listed below is the requested information as obtained from the literature since 1955.

ION	REACTANT	OTHER PRODUCTS	IP or AP	METHOD	YEAR	DOC NO
CN ⁺	CNI	I	18.1+0.1	SP	60	00073
CN ⁺	CNBr	Br	18.3+0.1	SP	60	00073
CN ⁺	CNC1	Cl	18.3+0.2	SP	60	00073
CN ⁺	CH ₃ NO ₂	?	19.15+0.09	IB	55	00090
CN ⁺	CH ₃ NO ₂	?	33.6+1.0	IB	55	00090
CN ⁺	CN		14.5+0.2	SP	61	00154
CN ⁺	CN		14.5+0.5	SP	61	00154
CN ⁺	C ₄ N ₂	C ₃ N	19.2+0.3	SP	61	00154
CN ⁺	HC=C-CN	C ₂ H	19.8+0.2	SP	61	00154
CN ⁺	C ₆ N ₂	C ₅ N	20.0+1.0	SP	61	00154
CN ⁺	(CN) ₂	CN	21.5+0.3	SP	61	00154
CN ⁺	cyclo-C ₃ H ₆ CN	C ₃ H ₆	19.5+0.4	EVD	62	00202

TERM DESIGNATION

SP=SEMILOG PLOT

IB=INITIAL BREAK

EVD=EXTRAPOLATED VOLTAGE DIFFERENCE

REFERENCES

00073 Herron, J.T. and Dibeler, V.H., "ELECTRON IMPACT STUDY OF THE CYANOGEN HALIDES", J.Am. Chem. Soc. 82, 1555(1960)

00090 Kandel, R.J., "APPEARANCE POTENTIAL STUDIES. II. NITROMETHANE", J. Chem. Phys. 23, 84(1955)

00154 Dibeler, V.H., Reese, R.M. and Franklin, J.L., "MASS SPECTROMETRIC STUDY OF CYANOGEN AND CYANOACETYLENES" J. Am. Chem. Soc. 83, 1813(1961)

00202 Kiser, R.W. and Hobrock, B.G., "THE IONIZATION POTENTIALS OF CYCLOPROPYL RADICAL AND CYCLOPROPYL CYANIDE", J. Phys. Chem. 66, 957(1962)

Please note that we make no claim that the above information has been critically evaluated by NBS personnel nor do we make any claim that there is a preferred value.

We hope that we may be of further assistance to you in the future.

Mass Spectrometry Section
Institute for Basic Standards
National Bureau of Standards
Washington, D. C. 20234

FIGURE 3. Print-out of data from NBS Mass Spectrometric Data Center, typical of uncritical-data compilation with bibliography.

Allowed Transitions

List of tabulated lines:

Wavelength [Å]	No.	Wavelength [Å]	No.	Wavelength [Å]	No.
687.059	10	3360.9	27	4413.2	24
687.35	10	3361.09	27	4618.9	26
687.355	10	3361.75	27	4628.1	26
858.092	9	3581.80	18	5132.96	14
858.559	9	3584.98	18	5133.29	14
903.624	3	3585.83	18	5137.26	14
903.962	3	3587.68	18	5139.21	14
904.142	3	3588.92	18	5143.49	14
904.480	3	3589.67	18	5145.16	14
1009.85	4	3590.87	18	5151.08	14
1010.07	4	3876.05	22	5640.50	13
1010.37	4	3876.19	22	5648.08	13
1036.34	2	3876.41	22	5662.51	13
1037.02	2	3876.67	22	5889.4	20
1065.88	6	3878.22	22	5889.97	20
1065.9	6	3879.60	22	5891.65	20
1066.12	6	3880.59	22	6578.03	11
1323.9	5	3881.2	22	6582.85	11
1334.53	1	3883.8	22	6779.74	12
1335.66	1	3918.98	17	6780.27	12
1335.71	1	3920.68	17	6783.75	12
2173.8	15	4074.53	23	6787.09	12
2174.1	15	4076.00	23	6791.30	12
2509.11	7	4267.02	21	6798.04	12
2511.71	7	4267.2	21	6800.50	12
2512.03	7	4267.27	21	6812.19	12
2746.50	19	4371.59	25	7231.12	16
2747.3	19	4372.49	25	7236.19	16
2747.31	19	4374.28	25	7236.2	16
2836.71	8	4411.20	24	18895	29
2837.60	8	4411.52	24	18916	29
2992.6	28				

Self-consistent field calculations by Weiss [1], and Biermann and Lübeck [3], and a high current arc experiment by Maecker [2] are utilized for the tabulation. The results for the lower and moderately excited transitions should be quite uncertain because in the calculations the strong effects of configuration interaction are essentially neglected, and the experimental work is subject to large systematic uncertainties.

References

- [1] Weiss, A. W., private communication (1964).
- [2] Maecker, H., Z. Physik **135**, 13-22 (1953).
- [3] Biermann, L. and Lübeck, K., Z. Astrophys. **25**, 325-339 (1948).

FIGURE 4. Illustrative page from Atomic Transition Probabilities, a critically evaluated compilation (Reference 2).

F. General Status of Program

The previous status report on the program of the Office of Standard Reference Data was issued in FY 1966 (Reference 3). At that time the principal data centers and lines of activity were well established and there has been little change of direction since. Nor has there been significant increase in level of effort; a slight increase in FY 1967 has been balanced by a slight decrease in FY 1968. Although this program has been assigned a high priority within NBS, overall budget increases have not been sufficient to permit expansion. (The small decrease in FY 1968 has been due to reduced participation by other agencies in the joint funding of projects.)

The status of the compilation projects can be briefly summarized as follows. The two general categories of "Thermodynamics and Transport Properties" and of "Atomic and Molecular Properties" have been judged to be of highest priority and have therefore received greatest attention. Significant progress has been made in these areas, as described in detail later. In "Nuclear Properties," only one project is supported by the NBS program. However, NBS staff members serve on committees of the Atomic Energy Commission concerned with data problems and good relations are well established. Small efforts continue in the areas of "Solid State Properties," "Chemical Kinetics," and "Surface and Colloid Properties;" the program has not developed in accordance with the plans of two years ago. The "Mechanical Properties" area has had only preliminary planning attention — no data projects have been started, and none are planned for fiscal years 1968 and 1969.

The Data Systems Design and Research activity has developed a variety of procedures and other software for use in data centers. These techniques are concerned both with data manipulation and with aiding rapid publication. A basic principle in this work is that the techniques must be usable by a clerk or secretary with little or no training in computer programming.

The Information Services Operation has been maintained at a rudimentary stage of development, since it has been decided that the largest possible fraction of available resources should be applied to the production of compilations and critical reviews. A monthly newsletter is published as part of the Technical News Bulletin of the National Bureau of Standards and is separately distributed to persons and institutions that have indicated a desire to receive it.^{1/} The Information Services Operation maintains an extensive collection of data compilations produced throughout the world and replies to a steadily growing stream of inquiries.

^{1/} A reader of this report who wishes to receive the NSRDS News regularly should send a request to Dr. Herman M. Weisman, Office of Standard Reference Data, National Bureau of Standards, Washington, D.C. 20234.

At the time of writing this report the procedures for marketing the products and services of the National Standard Reference Data System are being examined in some detail. The basic question is whether the National Bureau of Standards should be a retailer or a wholesaler in this field; that is, whether the NBS Office of Standard Reference Data should itself develop the mechanisms and capability to supply the needs of the individual user or should instead turn over its basic output to organizations such as commercial publishers, computer service companies, or industrial information systems which would then provide the interface with the individual user. Discussions are now being held with representatives of these various types of organizations to explore their views of their own roles and their relationships with NBS. A plan for future operation will be developed within the next few months.

G. International Cooperation in Standard Reference Data Activities

(1) Background — Evaluation and compilation of data on the properties of substances has been a joint activity of the world's scientists for many years. The International Critical Tables, produced mainly in the decade 1920-1930, contain contributions from scientists all over the world, coordinated through the efforts of the National Academy of Sciences. The Tables of Landolt-Börnstein, originally a German effort, now are produced through the cooperative participation of scientists from many countries. Indeed, in almost every developed country of the world, individuals have produced specialized compilations on various topics, many in cooperation with scientists elsewhere.

If appropriate cooperative arrangements can be worked out, the resulting comprehensive international program would have the advantages of sharing costs, getting the job done faster and better, and improving contacts among the scientists of the world.

Possible mechanisms for coordinating an internationally operated program include: (a) negotiating a series of informal bilateral agreements between cooperating countries, (b) cooperation through the recently established Committee on Data for Science and Technology of the International Council of Scientific Unions, (c) informal multilateral agreements among several cooperating countries, (d) cooperation under the aegis of an existing intergovernmental organization, such as OECD or UNESCO, (e) establishment of a new nongovernmental or intergovernmental organization specifically for the purpose, and (f) some combination of the preceding.

(2) Bilateral Activities — In the United Kingdom government responsibility for developing a program has been assigned to the Office of Scientific and Technical Information within the Department of Education and Science. This office has conducted a survey of existing activities and capabilities within the UK and is now supporting a number of projects after checking with NBS to determine that there was no conflict in plans.

In Germany the editors of the Landolt-Börnstein data compilations

and the management of the government-supported Gmelin Institute and Beilstein Institute have expressed considerable interest in the National Standard Reference Data System and have shown a desire to cooperate with the U.S. program. In addition, discussions have been held with representatives of the Deutsche Forschungsgemeinschaft and the Institute für Dokumentation. The Ministry of Science has also taken an interest in data compilation activities.

Under the U.S.-Japan Science Exchange Program, the Committee on Exchange of Information and Materials has discussed the initiation of a co-operative data compilation program. These discussions have not yet materialized into a plan of action.

In France, the Centre National de la Recherche Scientifique has for many years sponsored the production of the compilations Tables des Constantes et Donnees Numerique. The staff and financial resources are small at present. Discussions have been held with this group but no proposals for cooperative projects have been advanced.

The U.S.S.R. State System of Standard Reference Data (GSSSD) is a responsibility of the State Committee on Standards, under the general supervision of Professor Ivan I. Novikov, Deputy Chairman of the State Committee on Standards. During a recent visit to Moscow by the Chief of the NBS Office of Standard Reference Data, Prof. Novikov and other officials of the GSSSD expressed a desire to establish close relationships between the United States program and their own.

The technical scope of the Soviet program is broader than that of the U.S., including less well-defined properties of complex materials, customarily called "engineering properties," which are outside the U.S. National Standard Reference Data System. The technical areas receiving most emphasis in the U.S.S.R. are thermodynamics and transport properties and chemical kinetics, and numerous works are now in preparation.

(3) Foreign Currency Program — The Director of NBS has recently decided that the foreign currency (P.L. 480 funds) program operated by NBS should be concentrated in three program areas only, one of which is standard reference data. The Chief of the Office of Standard Reference Data was one of the members of a team that visited India, Pakistan, and Israel in January 1967 to explore the possibilities of developing a significant program in the areas of interest. As a result several interesting proposals have been received from institutions in India and Israel. Allocations of available funds are being decided at the time of writing this report.

(4) International Organization Activities — The International Council of Scientific Unions established in January 1966 a "Committee on Data for Science and Technology." This committee (called CODATA) has a directive to promote international cooperation, to serve as a channel of communication among projects in various countries all over the world, to encourage more scientists to undertake projects of this type, and to make recommendations about needs and priorities to persons responsible

for funding these kinds of projects in the various countries.

The second annual meeting of CODATA was held at the Headquarters of the Soviet Academy of Sciences in Moscow on May 31, June 1 and 2, 1967, under the Chairmanship of Frederick D. Rossini, Vice President for Research at the University of Notre Dame. The Chief of the Office of Standard Reference Data was invited to attend this meeting as an observer and was thereby enabled to learn about numerous data compilation activities in the U.S.S.R. and other countries.

Membership in CODATA consists of national representatives from the United States, United Kingdom, U.S.S.R., France, Germany, and Japan, plus representatives of those international scientific unions that wish to participate. The Committee is served by a full-time executive staff under the part-time directorship of Dr. Guy Waddington who also serves as Director of the Office of Critical Tables of the National Academy of Sciences-National Research Council.

The international scientific unions are, of course, nongovernmental organizations. Preliminary informal discussions have also been held regarding the desirability and feasibility of conducting an international standard reference data program under the auspices of an intergovernmental organization, such as OECD, or one of the United Nations specialized agencies, or a new agency created for the purpose.

* * * * *

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3. E. L. Brady, Ed., NBS Technical Note 289, Status Report, National Standard Reference Data System, April 1966 (Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402).

II. DATA SYSTEMS DESIGN AND DEVELOPMENT

During the year 1967 the staff of the Office of Standard Reference Data was augmented in order to accelerate plans to automate its own operations and to assist the various data centers to achieve similar objectives.

The Data Systems Design and Development group (formerly called "Information System Design and Research") is now composed of three professionals experienced in computer programming, systems design, and application, as well as data correlation. The DSD group's earlier experience gained in design and application of a number of general purpose computing programs like OMNITAB^{1/} is now providing guide-lines for the preparation of general-purpose computer programs for data storage and retrieval, for file manipulation, and for computer-assisted text preparation, editing and printing. In the latter area, the group is working in close collaboration with the Electronic Printing Section of the NBS Office of Technical Information and Publications in devising a variety of computer-based systems for more effective use of the Electronic Composing System at the Government Printing Office.

The work in this area can be grouped into three main activities:

- (1) Development of general-purpose computer programs required for the generation and updating of data files and the preparation of publications therefrom.
- (2) The design of computer-based data files and the retrieval systems to make them accessible to as wide a segment of the technical community as is economically possible.
- (3) Consultation and advisory services to the data centers adhering to the NSRD System.

Among the projects in which the Data System Design group is engaged or is promoting are the following:

(1) Computerized Data Files. The design and development of an experimental computerized file of Standard Reference Data for remote access via teletypes. This work will draw on the group's experience with a variety of time-shared computer systems. Efforts will be directed toward arranging the subject matter and the implementation to make the file attractive to university computing centers and to commercial groups offering

^{1/} J. Hilsenrath, OMNITAB, A Computer Program for Statistical and Numerical Analysis, NBS Handbook 101. Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402, Price \$3.

time-shared computer service to schools and colleges. It is planned to make the subject matter of the files of general use to teachers of physics and chemistry in teaching these subjects, hopefully thereby promoting feed-back on the utility, convenience, and economics of computerized data files.

(2) Computer-Assisted Text Preparation and Editing. The writing of general-purpose computer programs is continuing with the purpose of developing a system of compatible programs which will exploit the capabilities of the newest computer configurations. The programs and the subroutines they require are being written in ASA Standard FORTRAN IV. The use of a standard FORTRAN and other self-imposed restraints will make it easier to use the programs on a variety of machines.

The first release in this series is called EDPAC. It contains five programs that have been used extensively at NBS over the last two years. These are called JUSTIFY, SCRAMBLE, SEARCH, BLOCKSEARCH, and SUBSTITUTE.

The characteristics of EDPAC were outlined in some detail in the NSRDS Newsletter for December 1967. A list of applications of one of these programs (SUBSTITUTE) should serve to illustrate the extent of the generality that has been achieved. Among the diverse jobs to which SUBSTITUTE may be applied are the following:

- (a) Convert text punched on cards in BCD format (all capital letters) to upper and lower case, such as initial capitalization of the start of each sentence and authors' names and initials.
- (b) Replace any arbitrary set of symbols by corresponding instructions for a photocomposing machine.
- (c) Recognize typesetting instructions in a text and either delete them or replace them with other codes.
- (d) Anglicize text written by Americans (e.g., replace "program" by "programme").
- (e) Replace journal abbreviations by their five letter CODEN designations or vice versa, or by the full title.
- (f) Change citation numbers in the body of a paper to agree with a revised list of references.
- (g) Insert complex mathematical expressions when they occur frequently in a text, thereby avoiding needless retyping and subsequent proofreading.
- (h) Insert typesetting instructions in place of code words for special symbols not available on the input device.

- (i) Screen and correct automatically inconsistent use of abbreviations or symbols.

Other programs in varying stages of production are:

- (a) A general-purpose program for manipulating formatted data file.
- (b) A general-purpose program for editing structured but unformatted data files.
- (c) A program for automatic typesetting of computer-produced Key Word in Context (KWIC) indexes.
- (d) A program to generate indexes for books and reports.

(3) Automatic Typesetting and Composition of Data Tables. Valuable experience is being gained in writing computer programs to convert existing data tapes for automatic typesetting of NSRDS publications. An important consideration in this work is to design the programs in so far as possible for general rather than specific applications. While complete generality has not been achieved, the programs produced thus far do have wider applicability than to the document they have produced.

The experience gained in turning out about a half-dozen publications — more-or-less automatically — is encouraging enough for us to be optimistic that the conversion techniques will soon be simple enough so that each Data Center will be able to handle the file conversions themselves. This is in sharp contrast to the experience in the recent past when each book of tables required the services for a period of one or more months of a programmer experienced in both computing and typesetting.

The phrase, "more-or-less automatically," was used in the above paragraph because experience has shown that the most expeditious means for producing a finished product is to combine hand operations with computer-aided generations. One reason for our quick success in producing a number of data tables of complex structure is a decision to have the table captions and column headings handset and placed on a transparent film. The film is laid over each table, in turn, as the negatives are made.

One of the more perplexing problems to be coped with is that the grids presently available for the Electronic Composing System of the Government Printing Office do not have all of the characters required for the scientific text that accompanies our data tables. Sufficient experience has already been gained with the variety of characters required in NSRDS publications to form the basis for designing an appropriate set of grids. Until these grids are available, the Linofilm machine at the Government Printing Office will be used. In fact, both machines are expected to be used for some time to come. We foresee that some of the smaller jobs will continue to be set on the Linofilm.

(4) Input Devices and Line Printers. A major problem in the extension of computer techniques to the processing of scientific manuscripts — either for editing and automatic typesetting or for storage and retrieval — is the limited number of characters on the ordinary computer printer, card punch, and typewriter.

Recent developments in hardware and programming should soon provide a capability to handle text with scientific notations, such as subscripts, superscripts, Greek letters, mathematical and logic symbols, and diacritical marks present in some languages.

It is neither economical, nor necessary, for computer printers to provide authors with the nearly 1000 symbols available to printers who specialize in scientific publications. A computer line-printer component with 240 distinct characters and having provision for half-line spacings offers enough flexibility to cope with all but the most specialized situations.

In 1968, the Office of Standard Reference Data will have access to such a device. This line-printer will have 188 distinct characters, will be able to provide half-line spacing for subscripts and superscripts, and will be able to print several characters in the same position (e.g., / imposed over 0 gives Ø). (See NSRDS News, April 1968.)

While extended character printers have been in use for the past four years, they have not yet achieved their full potential. This results largely from the fact that the printing speed is reduced by having a greater variety of characters. Each group felt constrained, therefore, to limit the number of special characters. Thus, there is little if any compatibility between the existing extended character print chains trains or the software to support them.

The commercial availability of typewriter-like devices capable of communicating with computers over telephone lines in a standard code now makes it easier to define uniquely, and to transmit, a character set of 188 characters. The DSD group will shortly recommend a set of punching and keyboarding conventions for a variety of input devices ranging from key punches to keyboard-driven CRT display devices. A motivation for some of the general-purpose programs discussed above was to provide easy conversion from one punching or keyboarding system to another.

(5) Advanced Programming Languages. The group is continuing its contact with that segment of the computing profession which is involved in developing user-oriented systems, compilers, and languages that permit one to address the computer in a language closely related to the problem statement.

III. INFORMATION SERVICES

Limited financial resources of the Office of Standard Reference Data have severely inhibited the development of specific information services. Nevertheless, groundwork for services has been laid. Four basic units of activities for Information Services have been identified: (a) Data File, (b) Compilation Publication Services, (c) Inquiry Services, (d) Analysis and User Relations.

Data File. The initial task of this activity has been to acquire known world-wide data compilations and to organize the collection systematically. General planning of ultimate methods of indexing, storage, and retrieval has been begun. The Data File houses a collection of about 1000 reference data compilations.

Compilation Publication Services. This activity acts as an editorial intermediary between Office of Standard Reference Data associated data centers and other individuals and groups producing data compilations on the one hand, and publishers on the other hand, that is, the Government Printing Office, interfacing with the NBS Office of Technical Information. One of its functions is to produce the NSRDS News.

Inquiry Services. When resources are available, this unit will provide coordinated services for replies to inquiries from the Data File, from the Compilation Publication Services, from the associated data centers, and from other resources in the NBS. At present, if queries are within the capabilities and scope of the program, limited replies are being provided: sometimes inquiries are referred elsewhere, or reference sources are furnished, or copies of reference sources or data compilation or excerpts therefrom, or other publications are provided. Inquiries and requests increased from about 200 in the calendar year of 1966 to more than 400 in the calendar year of 1967. Most requests were for information on the NSRDS program or for copies of NSRDS publications. A few were for specific data points and/or information. Out of 419 requests, only 28 responses had to be negative because of lack of information or referral to a likely source of information.

Analysis and User Relations. The mission of this unit is to provide to the Office understanding of requirements, both present and future, of the NSRDS's actual and potential users. It also has the responsibility for providing the Office with information on how best to meet user needs and to develop feedback mechanisms to evaluate services provided.

Advisory Panel. An Advisory Panel on Information Services and Systems Design was organized. It met with the Office of Standard Reference Data in June 1966. A summary of major points of concurrence were:

- (1) That the Information Systems and Information Services Operations should evolve slowly, testing procedures and services as experience grows,

- (2) that the initial effort should be the preparation of compilations and dissemination of these into the hands of individual users as rapidly and as cheaply as possible,
- (3) that an attempt should be made as soon as possible, however, to design some form of mechanized storage and retrieval of information in order to gain experience and to develop techniques for the use of a system,
- (4) that the Inquiry Service should not be activated until the program is ready to handle subjects covering a wide area, or at least within a specific area to be ready to handle any questions or inquiries that might be addressed to it, and
- (5) that user surveys be regarded with great circumspection.

NSRDS News. The program's monthly newsletter was established in June 1966. It first appears as a special section of the NBS Technical News Bulletin and then is reprinted separately and sent to more than 3200 interested individuals. Regular features include an updated list of publications from the National Standard Reference Data System and descriptions of the program's data centers and compilation projects, as well as other items of news.

Machine-Readable Scientific Text. A "General Purpose Scientific Document Image Code" has been developed as the central component of a system for mechanizing the processing and exchange of scientific information in machine readable form. Such a system is needed by the data and information centers supported by the Office of Standard Reference Data. In this system a scientific typescript, with all its traditional complex symbolism and highly structured page format, may be transferred to digital machine form with virtually no limitations on the notation that may be employed. (See April 1968 NSRDS News.)

An attempt was made in the design of the system to assure broad applicability by emphasizing (a) exchange of information via telecommunication devices compatible with the American Standard Code for Information Interchange, (b) design of hardware to permit use of the proven skills of ordinary scientific typists in the record capture process, (c) exploitation of the capabilities of commercially available extended character high-speed line printers for direct computer output, and (d) publication using this type of machine record as the "typescript" input to computerized typesetting programs.

This system was developed in the NBS Physical Chemistry Division, and is being tested on records produced by the Chemical Kinetics Information Center and the Chemical Thermodynamics Data Group located there. To date two prototype "taxywriters" (type-augmented x-y recording typewriters) have been built. Computer programs for the input, editing, and retrieval of records have been written and tested on a pilot plant scale. Tests indicate that the System will be readily adaptable to other data collection operations.

Discussion Forum, Data and Information Center Operators. A meeting of all data and information center operators associated with the Office of Standard Reference Data was held April 6-7, 1967, at NBS. Representatives of 18 data and information centers within NBS and 10 centers outside the Bureau participated in the Forum. The major objectives of the meeting were: (a) to examine and develop machinery for communication exchanges and work sharing, (b) to explore means for establishing compatibility among operational procedures of the centers, (c) to explore and help formulate standards of quality, and (d) to define relationships between and among the Office of Standard Reference Data and associated centers and to develop machinery for more effective aid to centers.

General reaction to the Forum was as follows:

- (1) All center directors considered the Forum worthwhile and fulfilling the listed objectives.
- (2) Most center directors were either in favor of a centralized bibliographic service or willing to explore the feasibility for their needs.
- (3) Practically all centers wished the Office of Standard Reference Data to serve as a clearinghouse on information of useful methodologies, practices, and other matters of interest.
- (4) Centers were about evenly divided in their opinion as to whether the Office of Standard Reference Data should develop a file of standard reference data within the data banks of associated centers for mechanized relay of data and information to a requesting center.
- (5) There was a similar even division of opinion on the question of the Office of Standard Reference Data serving as a centralized inquiry service for all associated centers on questions from the technical community.
- (6) Most centers were willing to explore mechanization of their procedures, especially computer-aided composition of publications.

Survey on Data Needs. The Office of Standard Reference Data in cooperation with Industrial Research magazine conducted a survey in the magazine's May 1967 issue to determine:

- (1) Data and information needs of scientists and engineers within the industrial research community.
- (2) How such needs are now met.
- (3) Patterns of use of data, information, and reference sources.
- (4) Problems in finding required data and information.

Results of the survey show:

- (1) That of about 600 scientists and engineers responding, 75 percent experience problems in locating or obtaining materials properties data.
- (2) During a typical week, 55 percent of the respondents must look up properties data from 1-5 times. Among others, the task is more demanding -- occurring 6-10 times for 22 percent and more than 10 times for 19 percent.
- (3) Generally it takes less than an hour for the majority to locate the necessary information. However, 24 percent spend from 1 to 8 hours; and 8 percent normally search for days or weeks.

Among other items of interest the survey revealed was:

- (1) The printed book is the most frequently used and preferred form of data in use by the respondents.
- (2) Seventy-two percent of the respondents require and use bibliographies.

The survey showed that 82 percent of the respondents were engaged in research and development; 17 percent in manufacturing and processing. The disciplines represented were: 37 percent in chemistry; 32 percent in engineering; 12 percent in physics; 8 percent in the life sciences; the rest divided among miscellaneous groupings.

Almost from the start of the applications of nuclear physics twenty-five years ago, for both historical and practical reasons, a great deal of effort has been expended in the compilation and evaluation of nuclear data. The Atomic Energy Commission, from its inception, has encouraged through its operating divisions the support of data activities. The figure at the end of this section summarizes lines of direct responsibilities from major data centers to their sponsoring agencies. The dashed lines indicate advisory roles or cooperative activities. Especially noteworthy is the degree of cooperation active or anticipated between data centers on either side of the Atlantic Ocean.

Since the previous Status Report, two major undertakings in this field have come to fruition. The first is the publication of a journal, in two sections, Nuclear Data, edited by Dr. Katharine Way, which provide a mechanism for the dissemination of appropriate compilations or evaluations of nuclear data. Three volumes of Section A of this journal have appeared already. Section A contains a wide variety of types of information — e.g., a set of evaluated data for a single element or charged particle cross section data for many elements; Section B of the journal, of which two volumes have appeared, is the publication mechanism for the data sheets of the Nuclear Data Project of the Oak Ridge National Laboratories, which previously were published in loose-leaf or pamphlet form.

A second major development is the reorganization of neutron data compilation and evaluation activities centered at Brookhaven National Laboratory. For some time there has existed a Cross Section Evaluation Center (CSEC) in parallel with the Sigma Center. These two centers have been combined into the National Neutron Cross Section Center (NNCSC) with responsibilities as described below.

The following two sections comprise a list of continuing nuclear data centers with brief summaries of their activities. A more complete description of these activities is available in the COSATI-sponsored Directory of Federally Supported Information Analysis Centers. The order chosen is consistent with the Figure 5, reading left to right.

I. Nuclear Data Centers in the United States

A. Photonuclear Data Center, National Bureau of Standards, E. G. Fuller, Director. This center provides bibliographic information and the best available data for photonuclear reactions of all nuclei. This center is wholly supported by the Office of Standard Reference Data; its operation is described in more detail at the end of this section.

B. Applied Science Data Group at the Lawrence Radiation Laboratory at Livermore, R. J. Howerton, Director. In the past, reports containing neutronic and photonic evaluated cross section data have been

disseminated by this group. Recently, they have expanded their interest to include the general problem of information storage and retrieval.

C. Radiation Shielding Information Center at Oak Ridge National Laboratory, D. K. Trubey, Director. Provides information and computer programs, including appropriate nuclear data, for all aspects of shielding problems: reactors, weapons, radioisotopes, accelerator, and space problems.

D. Argonne Code Center, M. Butler, Director. A depository for all computer programs associated with the design of nuclear reactors and an analysis of the performance of the reactors.

E. Reactor Physics Constants Center at Argonne National Laboratory, R. Avery, Director. This center supplies those "integral" physical quantities which are of direct need in reactor physics calculations. The product has taken the form of two editions of a collection of reviews entitled, "Reactor Physics Constants" (ANL-5800), and an assortment of newsletters.

F. National Neutron Cross Section Center, Brookhaven National Laboratory, S. Pearlstein, Acting Director.

(1) Sigma Center, M. Goldberg, Director. In previous years, this center compiled neutron cross section data which were published periodically as the familiar Barn Books (BNL-325 for total cross section data and BNL-400 for angular distributions). Recently, all available neutron cross section data have been stored on a computer library tape and it is now possible to have access to the compiled data by direct communication between the user and storage tape.

(2) Cross Section Evaluation Center, S. Pearlstein, Director. The original function of this center was to provide a set of evaluated neutron cross sections for all important nuclides over the entire range of energies of importance for reactor purposes, i.e., from approximately one millivolt to 15 MeV. With the assistance of a group of evaluators who formed the Cross Section Evaluation Working Group working in laboratories throughout the country, a set of such cross sections, together with auxiliary computer programs for the appropriate manipulation of these data points, has recently been completed. This set of cross sections is designated the Evaluated Nuclear Data File. Recently, the purview of this center has been broadened to include neutron cross sections of interest for application to systems other than reactors.

G. Nuclear Data Group, Oak Ridge National Laboratory, K. Way, Director. This group publishes nuclear data sheets containing data on nuclear level properties organized according to nucleus.

H. Charged Particle Cross Section Information Center at Oak Ridge National Laboratory, F. K. McGowan, Director. Compiles nuclear cross-section data for charged-particle-induced reactions.

I. Berkeley Elementary Particle Center, M. Rosenfeld, Director.

Compiles and evaluates data on elementary particles and their interactions.

J. Division of Technical Information Extension, Oak Ridge. This organization has for many years published Nuclear Science Abstracts. Recently, it has assumed responsibility for the publication of "CINDA," a computer based annotated bibliography of all neutron cross section information. CINDA was originated by H. Goldstein of Columbia University, and now is produced through international cooperation, as described below.

The following activities do not appear on Figure 5, but are related:

K. Energy Levels of Light Nuclei, compiled by F. Ajzenberg-Selove and T. Lauritsen. This compilation is concerned with nuclei with atomic weights less than or equal to 20. A new edition is under preparation, with a portion, A=5-10, published.

L. Table of Isotopes. The Sixth Edition of this continuing work has recently been published in book form by C. M. Lederer, J. M. Hollander, and I. Perlman, of the Lawrence Radiation Laboratory, Berkeley. It was originated by G. T. Seaborg and includes much of the information available on the Nuclear Data Sheets, but with briefer annotation.

M. Chart of the Nuclides. The Ninth Edition of this familiar wall chart of the property of nuclides was published by the General Electric Company and prepared by D. T. Goldman and J. R. Roesser.

N. Scintillation Spectrometry Gamma-Ray Spectrum. The compendium of experimental measurements is brought up-to-date periodically by R. L. Heath of the Idaho Nuclear Corp., who is also responsible for most of the data contained therein. Recently the group was augmented by the addition of R. C. Greenwood, who with J. H. Reed, published "Prompt Gamma-Rays From Radiative Capture of Thermal Neutrons," IITRI-1193-53 (Vols. 1 and 2) (1965).

As indicated in the ensuing diagram, there presently are lines of communication and some support between parts of the Atomic Energy Commission and other governmental agencies. It is anticipated that such cooperation will grow as more activities of mutual interest are recognized.

II. Data Centers Outside the United States

A. The Neutron Data Compilation Centre at Gif-sur-Yvette, France. This center is sponsored by the European Nuclear Energy Agency and its present chief is V. J. Bell. Its major activity is the compilation of neutron data from the thirteen OECD countries and the exchange of information between data centers in other parts of the world. This center is one of the contributors to and publishers of the CINDA Index. In addition, it maintains a computer library of neutron cross sections which is compatible with the Sigma Center file. Data evaluations are published from time to time in the Centre's Newsletters.

B. The Nuclear Codes Center at Ispra, Italy, J. Rosen, Director, maintains a file of computer programs of use in both reactor design and shielding applications.

C. The Central Bureau of Nuclear Measurements at Geel, Belgium, has sponsored the compilation of certain neutron reactions such as (n,p) , (n,α) , and $(n, 2n)$. A report has been published by H. Lisskien and A. Paulsen, with this compilation. In addition, other compilations will be undertaken.

D. A similar sort of operation to that described above is performed in Sweden under the sponsorship of A. B. Atomenergi and the Research Institute of National defense. Reports such as Cross Sections for Neutron Inelastic Scattering and $n, 2n$ Processes, A Review of Available Experimental and Theoretical Data, by M. Leimdorfer, et al, and the Optical Model of the Nucleus, an Index and Abstracted Literature Review, by L. Wallin, et al, have been published.

E. Nuclear Data Unit, International Atomic Energy Agency, Vienna, Austria, W. Good, Head. This group is attempting to provide the kind of services for the remaining countries that the CCDN provides for OECD nations. It is listed as one of the publishing organizations of the most recent edition of CINDA. A particularly useful evaluation of the thermal neutron cross sections of fissile nuclei was performed by this unit and published under the leadership of C. Westcott.

The following activities do not appear on the Figure, but are of sufficient interest to be noted:

F. U.S.S.R. Nuclear Data Information Centre at Obninsk, A. Abramov, Director. This center is also one of the contributing publishers of CINDA 67.

G. A Nuclear Cross Section Evaluation Activity has been undertaken for several years in the United Kingdom jointly by the Atomic Weapons Research Establishment, Aldermaston, under the direction of K. Parker and E. Pendleburg, and the Atomic Energy Establishment, Winfrith, directed by J. S. Story. A large library of evaluated cross sections is available.

H. Kernforschungszentrum, Karlsruhe, Germany, J. J. Schmidt of this laboratory, has undertaken the systematic evaluation of neutron cross sections for many elements and has recently published a very lengthy document containing them, "Neutron Cross Sections for Fast Reactor Materials, Part I: Evaluation," KFK120 (1966).

I. Mainz-Amsterdam. J. Mattauch of the Max Planck Institute for Chemistry in Mainz and A. Wapstra of Amsterdam have, for several years, issued a list of atomic masses prepared by a detailed evaluation of the available experimental data for a variety of nuclear reactions in addition to direct mass spectrometric measurements. In addition, Dr. Wapstra has compiled energy levels of very heavy nuclei, that is, nuclei heavier than those presently treated in the Nuclear Data Sheets.

J. Utrecht, Netherlands. Professor P. Endt and associates for several years have been compiling and publishing information on the

energy levels of light nuclei for Z=11 to Z=20. This work includes the same information as the compilation listed in I.K. above, but for somewhat heavier nuclei.

K. Vienna-Dresden. W. Kunz (Vienna) and J. Schintlmeister (Dresden) have begun publishing a series of volumes containing nuclear reaction data and nuclear energy levels. These are compiled from original literature and thus far two volumes have appeared under the general heading, "Nuclear Tables; Part II: Nuclear Reactions," Vol I. "The Elements From Neutron to Magnesium," and Vol. II, "The Elements From Aluminum to Sulfur."

III. International Cooperation

In the field of nuclear data, cooperation between different countries has a history about as long as the field itself. At present, a variety of formal agreements and informal arrangements have contributed to mutual cooperation and the avoidance of duplication of activities. International committees exist to provide communication links among laboratories in many countries. The direct cooperation between data centers has already been described. The computer program exchange activities of the Ispra Code Center and the Argonne Code Center and Radiation Shielding Information Center at Oak Ridge has been in existence for several years. The CINDA annotated bibliography has furnished a concrete example of multinational cooperation. Many countries have representatives on the International Nuclear Data Committee, an advisory group to the International Atomic Energy Agency, which was responsible for the establishment of the Nuclear Data Unit in Vienna. Neutron cross section data tapes have been prepared jointly by the Brookhaven and ENEA Data Centers. The Joint Subcommittee on Nuclear Data Evaluation has provided discussion opportunities on this subject as well as providing the impetus for a joint European-American compendium of neutron data evaluations.

Further examples of cooperation are evident at international conferences. The initial meeting of neutron data evaluators from the U.S. and OECD in Brookhaven in 1965 was followed by an IAEA Conference on Nuclear Data for Reactors in Paris, 1966 and a forthcoming Neutron Cross Sections and Technology Conference as well as frequent ICSU sponsored international meetings.

IV. Office of Standard Reference Data Nuclear Data Projects

Title: Compilation and Evaluation of Photonuclear Data

Location: Radiation Physics Division, IBS, NBS

Principal Investigator: Everett G. Fuller

Date Initiated: January 1, 1963

Technical Scope: This center is concerned with abstracting, compiling, indexing, and evaluating the published experimental data on the interactions of high energy electromagnetic radiation with nuclei. The primary

objective of the center's work is to maintain an up-to-date file of data in the field of photonuclear reactions as well as to publish periodically an annotated index to these data. In addition, a systematic evaluation of the data is to be made and published as a series of monographs or review articles covering selected groups of nuclei. The data are of particular interest for the fields of nuclear physics, astrophysics, analytical analysis, radiation processing and treatment, and radiation shielding. Close contact is maintained with other nuclear data compilation and evaluation groups supported by the AEC.

Properties and Species: Total photon interaction cross sections, cross sections for specific photon induced reactions ((γ, n) , (γ, p) , (γ, γ) , etc.), spectra and angular distribution of photodisintegration reaction products, inverse capture reactions ((p, γ) , (n, γ) , (d, γ) , etc.), inelastic electron scattering cross sections, Q-values for photonuclear reactions, abundances of stable isotopes. Cross section data are abstracted and filed for all stable nuclei and for nuclear excitations primarily but not exclusively in the energy range from 5 to 150 MeV.

Products Issued: (a) NBS Miscellaneous Publication 277, Photonuclear Data Index (covering period from 1955 through 1964), issued April 1, 1966, (b) NBS Miscellaneous Publication 277, Supplement 1, Photonuclear Data Index (covering period from January 1965 through April 1967), issued October 1967.

Status of Work: The data file is being maintained current to within about 3 months with the published literature. The first supplement to Miscellaneous Publication 277, Photonuclear Data Index, has been published (October 1967). This supplement includes listings of data published as late as April 1967, a delay of only six months compared with the sixteen month delay between the last reference and the publication date of the original index. Work has started on the evaluation of the available data on the s- and p-shell nuclei.

Future Plans: The data file will be maintained current with the newly published material in the field. It is expected that a critical review will be completed of the available data in the s-shell nuclei and published either as a monograph or review article. Unless shortages of personnel prevent it, a similar review should be completed for the p-shell nuclei.

Comments: In connection with the evaluation activities mentioned above, the original data available only in graphical form will have to be digitized. This will be carried out manually at first. At the same time, if budgetary and personnel limitations permit, various computerized techniques for the digitizing, analysis, and storage of data will be investigated. Work will be carried out aimed at developing some type of computerized system to handle all aspects of the data center's activities. This includes: library functions for data, index material, and bibliographical information; production of copy for publication of complete data index or of selected portions of the complete index along with the appropriate reference list; comparison and analysis of data from various sources.

Flow Chart Outlining the Administration of
Nuclear Data Compilation and Evaluation Activities

The following are abbreviations used in the accompanying chart. Listed in parentheses are the locations of the organizations and cognizant individuals, listed for identification purposes (reading from left to right).

NBS	National Bureau of Standards
OSRD	Office of Standard Reference Data
PNDC	Photonuclear Data Center (E. Fuller)
DOD	Department of Defense
DASA	Defense Atomic Support Agency
USAEC	United States Atomic Energy Commission
DMA	Department of Military Applications
LRL	Lawrence Radiation Laboratory, Livermore (R. Howerton)
DRDT	Division of Reactor Development and Technology
ACRP	Advisory Committee on Reactor Physics
RSIC	Reactor Shielding Information Center (D. Trubey)
RPCC	Reactor Physics Constants Center (R. Avery)
ACC	Argonne Code Center (M. Butler)
NNCSC	National Neutron Cross Section Center
CSEC	Cross Section Evaluation Center (S. Pearlstein)
CSEWG	Cross Section Evaluation Working Group
ENDF	Evaluated Nuclear Data File
Σ -Center	Sigma Center, Brookhaven (M. Goldberg)
DR	Division of Research
NCSAC	Nuclear Cross Section Advisory Committee
NDG	Nuclear Data Group, Oak Ridge (K. Way)

Abbreviations Continued -

CPCSC	Charged Particle Cross Sections Center (F. McGowan)
BPDC	Berkeley Particle Data Center
DTI	Division of Technical Information
DTIE	Division of Technical Information Extension, Oak Ridge
NSA	Nuclear Science Abstracts
CINDA	Computer Index of Neutron Data
AEC,L	Atomic Energy of Canada, Ltd.
OECD	Organization for Economic Cooperation and Development
ENEA	European Nuclear Energy Agency
EACRP	European-American Committee on Reactor Physics
EANDC	European-American Nuclear Data Committee
JSNDE	Joint Subcommittee on Nuclear Data Evaluation
CCDN	Centre de Compilation de Donnees Neutronique, Saclay
NCC	Nuclear Code Center, Ispra (J. Rosen)
CBNM	Central Bureau for Nuclear Measurements (J. Spaepen)
IAEA	International Atomic Energy Agency
INDCSWG	International Nuclear Data and Cross Section Working Group
NDU	Nuclear Data Unit, Vienna (W. Good)
A.O.	Atlantic Ocean

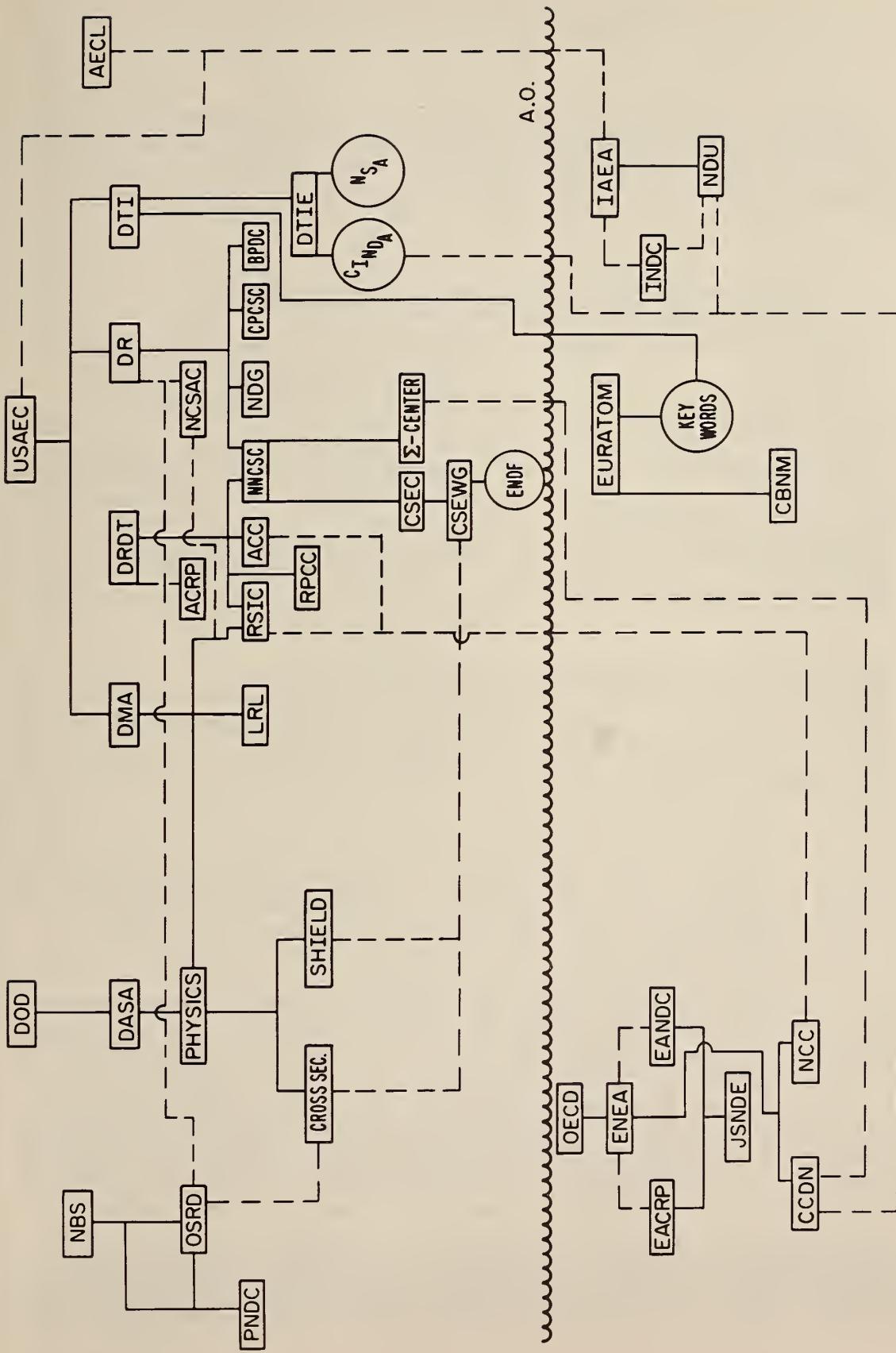


FIGURE 5. Flow Chart Outlining the Administration of Nuclear Data Compilation and Evaluation Activities.

V. ATOMIC AND MOLECULAR PROPERTIES

The Atomic and Molecular Properties area encompasses primarily properties characteristic of individual atoms or molecules rather than of substances in any specific state of aggregation. A more explicit indication of the scope of this area is given below in the list of major property topics.

MAJOR TOPICS IN ATOMIC AND MOLECULAR PROPERTIES

Fundamental constants and properties	Information on molecular energy levels derived from spectral data — diatomic molecules
Atomic energy levels	Information on molecular energy levels derived from spectral data — polyatomic molecules
Atomic spectral data	Other well-defined properties of atoms and molecules
Atomic and molecular X-ray spectral data	Transition probabilities
Atomic and molecular collision data	Computed functions
Particle-surface interactions	Interatomic and intermolecular forces
Plasma properties	
Direct spectral data	

Reference data on Atomic and Molecular Properties find application in two broad categories — basic scientific research and the extension of theoretical understanding on one hand, and technological problems, including analysis and identification of substances on the other.

General guidance for the Atomic and Molecular Properties program is provided by an advisory panel headed by Dr. E. U. Condon of the University of Colorado. This panel met first in May 1965 at Boulder, Colorado and again in May 1967 at the National Academy of Sciences in Washington, D.C. At the outset, the advisory panel recognized that additional close attention would be necessary in several areas, and that subpanels of specialists in the individual topics could appropriately be convened to consider needs. It was anticipated that there would be only slight overlap between membership on the advisory panel and membership on the subpanels.

Three specialized advisory groups have met so far: (a) The continuing advisory body on infrared spectroscopy is the Board of Management of the Coblentz Society. This group has met several times at the request of

the Office of Standard Reference Data to provide advice and guidance of several sorts. One of its specific tasks, to prepare criteria for the evaluation of infrared spectra, is described in more detail below as a program element. In addition, the Board has given advice on the development of infrared spectral data compilation projects at various quality levels. (b) An ad hoc advisory group on NMR spectroscopy, organized by Dr. B. L. Shapiro, met in November 1967 in Washington, D.C. to discuss data needs and possible compilation projects on chemical aspects of NMR spectroscopy. (c) An ad hoc panel on the application of computers to spectral information was convened on July 24 and 25, 1967, with Dr. E. R. Lippincott as Chairman. In addition to recommendations to the Office of Standard Reference Data, this panel provided discussions leading to a U.S. presentation at the 9th European Congress on Molecular Spectroscopy, held under IUPAC sponsorship in Madrid, September 10-15, 1967.

The Atomic and Molecular Property List developed in May 1965 was revised in 1967. Fifty-seven specific topics are now included, and thirty-four of these have high-priority ratings. Twenty of the thirty-four are receiving some compilation or planning attention under NSRDS programs (in some cases, a single project covers several items). Projects under other sponsorship are covering five topics. In addition, several of the most important items, such as molecular spectroscopic data, are being considered by two or more projects at the same time. The Office of Standard Reference Data tries to coordinate such multiple coverage, and to eliminate undesirable duplication of effort.

Most of the projects in the Atomic and Molecular Properties area have already produced valuable publications. So far eight compilations of data have been published in the NSRDS series, plus two which appeared in Reviews of Modern Physics. Eleven specialized bibliographies have been published, as have one set of criteria for evaluation, and two directories of workers in specialized fields. Nine compilations of data were in various stages of publication as of December 31, 1967. Six of these were due to appear in various NBS series, two in scientific journals, and one through a commercial publisher. Identification of all these products is given below.

Two projects listed in the 1966 Status Report have been closed out with the completion of their task and the publication of their material as NSRDS-NBS-10, Selected Values of Electric Dipole Moments for Molecules in the Gas Phase, by R. D. Nelson, Jr., D. R. Lide, Jr., and A. A. Maryott, and NBS Miscellaneous Publication 281, Bibliography on Flame Spectroscopy, by R. Mavrodineanu. One project, started since the last Status Report, has already completed its task and is being closed out. Its product, Compendium of ab initio Calculations of Molecular Energies and Properties, by M. Krauss, has been published as NBS Technical Note 438. The abstract of Technical Note 438 is given below, as a description of the work and its product.

Several of the projects listed below are supported by the Advanced Research Projects Agency of the Department of Defense, under an arrangement which provides for joint contributions by NBS and ARPA to coverage

of selected topics of common interest. In addition, the Atomic Energy Commission joins NBS in supporting the Atomic and Molecular Processes Information Center.

The project descriptions which follow were prepared, in the most part, by the individual principal investigators or project leaders. Further details and indications of progress can be obtained by writing to the Office of Standard Reference Data or the person in charge of the project.

1. Title: Diatomic Molecule Spectra and Energy Levels Data Center

Location: Heat Division, NBS

Principal Investigator: A. M. Bass

Date Initiated: July 1966

Technical Scope: This activity concentrates on the data of diatomic molecular spectra. Such data as wavelengths of characteristic bands in the electronic spectra of diatomic molecules, energy levels associated with observed transitions, spectroscopic constants for observed states, potential energy curves, and so forth, are of great importance in the many situations involving interactions of diatomic molecules. Although in the past some efforts have been made to summarize the data at a particular time (the most notable collection being the extensive tables in Herzberg's "Spectra of Diatomic Molecules," which compiled data as of 1950), it is believed that a need exists for a data compilation activity on a continuing basis.

Properties and Species: Spectroscopic data for all diatomic molecules; diatomic molecule properties which may be determined directly from optical spectroscopic observations. These data include wavelengths and intensities for all reported transitions, energies, ionization potentials, etc.

Products Issued: P. H. Krupenie, "The Band Spectrum of Carbon Monoxide," NSRDS-NBS-5 (1966). P. H. Krupenie and W. Benesch, "Electronic Transition Moment Integrals for First Ionization of CO and the A-X Transition in CO^+ . Some Limitations on the Use of the r-Centroid Approximation," submitted for publication in a scientific journal.

Status of Work: As a preliminary to later work on critically evaluated data, we have undertaken to assemble a complete bibliography of the published literature on diatomic molecule spectra through the year 1966. The bibliography, when complete, will be stored on punched paper tape to facilitate retrieval and reproduction. The reference material will be maintained at the Data Center where it will be used for preparing reviews and compilations. The published literature is being surveyed on a continuing basis, and the bibliography will be kept current.

A report on the band spectrum of the oxygen molecule (similar to previously published report on carbon monoxide) is being prepared. It is anticipated that the oxygen report will be completed by July 1968.

Future Plans: For the next year major emphasis will be placed on completion and publication of the bibliography of diatomic molecule spectra.

Plans are being made for the compilation of a far ultraviolet molecular band atlas. Such a compilation will be of increasing value as the level of research effort in the vacuum ultraviolet is expanded.

2. Title: Data Center for Atomic and Molecular Ionization Processes

Location: Physical Chemistry Division, NBS

Principal Investigator: H. M. Rosenstock

Date Initiated: January 1965

Technical Scope: The purpose of this program is to collect numerical data on the energetics of gaseous ionization. This includes ionization potentials, appearance potentials, and the properties of excited ionic states.

These data are required by workers in many fields including mass spectroscopy, chemical kinetics, and astrophysics.

Properties and Species: Ionization and appearance potentials of all atomic and molecular species. Heats of formation of ions at 298 K (in collaboration with J. L. Franklin, Rice University).

Products Issued: "A Bibliography on Ion-Molecule Reactions, Jan. 1900 to March 1966," NBS Technical Note 291, June 1966. "Two National Bureau of Standards Data Centers: Chemical Kinetics and Mass Spectrometry," (in collaboration with Dr. D. D. Garvin) J. Chem. Doc. 7, 31 (1967).

Status of Work: (a) Literature from 1955 through June 1966 abstracted and about 6000 sets of numerical data entered on punch cards. (b) Data have been evaluated and ionic heats of formation calculated in conjunction with J. L. Franklin, Rice University. (c) The data are now being ordered and corrected in a form suitable for publication. Target date is early 1968.

Future Plans: The literature published since June 1966 is to be abstracted and the numerical compilation brought up to date.

Comments: Requests for specific information by individuals in government, industrial, and academic laboratories are being answered on a same-day basis.

3. Title: Molecular Fundamental Vibrational Frequencies

Location: Department of Chemistry, University of Tokyo, Japan

Principal Investigator: T. Shimanouchi

Date Initiated: July 1, 1964

Description of Project: Compilation of vibrational frequency data for selected polyatomic molecules is conducted on a continuing basis. Vibrational frequency data are not only useful in research on molecular structure, but are also essential to accurate computation of ideal gas thermodynamic properties. They have proved highly valuable as well to those who employ infrared or Raman spectra in analytical applications.

Tables are issued (on a yearly schedule) for selected and related molecules, with special attention to successive degrees of deuteration and to inclusion of structural sources. Fundamental frequency and assignments are adopted only when they are definitely supported by the calculation of normal vibrations based on a consistent set of force constants which correlate the frequencies of molecules having similar structures.

Properties and Species: Fundamental vibrational frequencies of molecules. For each molecule, $(3N-6)$ values are given where N is the number of atoms in the molecule. The tables include also assignments to modes of vibration, identification of reliability and probable error, and the infrared, Raman, and other sources of information from which the frequencies are obtained. It is planned that the series of tables will cover a representative and comprehensive selection of basic molecules starting from H_2O , NH_3 , and CH_4 , and ending with high polymers.

Products Issued: NSRDS-NBS-6, "Tables of Molecular Vibrational Frequencies, Part 1," NSRDS-NBS-11, "Tables of Molecular Vibrational Frequencies, Part 2," and NSRDS-NBS-17, "Tables of Molecular Vibrational Frequencies, Part 3."

Status of Work: Part 4 (about 50 molecules) is now being prepared. The manuscript of a consolidated volume including the first 229 molecules of Parts 1, 2, 3, and 4 is also being prepared.

Future Plans: Data of this type are needed for several hundred key molecules. Uniformity of treatment is very important. The project will be continued for several years.

4. Title: Evaluation and Publication of Data From the Published Literature on Thermodynamic Properties of Ions

Location: Rice University, Houston, Texas

Principal Investigator: J. L. Franklin

Date Initiated: November 1, 1965

Description of Project: The objective of this project was to accumulate all of the data in the literature since 1955, when the last previous compilation was published, on the appearance potentials, ionization potentials, and related data on ions in gases. This program enjoyed the collaboration of the Mass Spectrometry Section of the National Bureau of Standards, who were primarily responsible for recovering the data from the literature, and of Dr. Frank H. Field of Esso Research and Engineering Company, who participated in the evaluation of the data and in some of the editorial work.

Properties and Species: The principal information obtained directly is appearance potentials of gaseous ions measured by electron impact, photoionization, photoelectron spectroscopy, and vacuum ultraviolet spectroscopy. From these data heats of formation of the gaseous ions have been calculated. From the heats of formation thus calculated and from various considerations of the validity of the methods, "best" values for each ionization potential have been selected and estimates of the accuracy of the data have been made. The literature covered was that from 1955 through June 30, 1966; positive ions only are covered.

Products Issued: This compilation of ionization potentials is now in press.

Status of Work: The program thus far has been devoted to the data on positive ions published between 1955 and June 30, 1966. The first phase of the program is complete, except for the final transmission of the tabulated material to the printer and some editorial work. Beyond that, only proofreading and similar editorial activities are involved.

Future Plans: It is planned to prepare an addendum to the first compilation to complete the data on positive ions from July 1, 1966 to Dec. 31, 1967. Subsequently, we would plan to accumulate and evaluate the data in the literature on negative ions from 1955 forward. The latter, while involving less data, will be more difficult to accumulate because of the wider range of techniques and information sources involved. In the future, it is hoped to issue supplements containing recent information on positive and negative ions and from time to time as developments justified, to reissue complete compilations.

Comments: The data on thermochemical properties of gaseous ions are broadly useful in various aspects of mass spectrometry and in the interpretation of data concerning electric discharges, flames, radiation chemistry and, in many instances, solution chemistry. The data are widely distributed in the literature and are difficult both to recover and to appraise. Continuing collection and evaluation of these data make a valuable contribution to progress in the above fields.

5. Title: Compilation of Semi-empirical and Approximate Theoretical Molecular Calculations

Location: Georgetown University, Department of Physics

Principal Investigator: W. L. Clinton

Date Initiated: April 1, 1967

Description of Project: In the initial phase of this project, the principal investigator undertook to survey, analyze and review critically the "non-ab-initio" areas of quantum mechanical computations as applied to atoms and small molecules. A bibliography of the literature and a detailed review were intended as the principal products. As the work progressed, it became apparent that the detailed review, which took the form of specific compilation sheets on individual topics with digest of each topic, should be supplemented with a general summary and an overall state-of-the-art analysis.

Properties and Species: All properties which are subject to theoretical computation and which are reported in the literature, for diatomic molecules, with the inclusion of some small polyatomic and atom data.

Products Issued: None.

Status of Work: The initial bibliography, covering the period 1955-1967, has been delivered to the Office of Standard Reference Data in the form of computer printout. The detailed critical review is in manuscript form, and is being typed for submission for publication. Work on the general summary has been begun, and the bibliographic coverage is currently being extended through September 1968.

Future Plans: Complete bibliographic coverage through September 1968 at least, put all compiled material into machine-readable form; publish detailed critical review material; complete and publish general summary.

Comments: A general review paper in this area is urgently needed.

6. Title: Atomic Energy Levels Data and Information Center

Location: Atomic Physics Division, NBS

Principal Investigator: Charlotte M. Sitterly

Date Initiated: 1946

Description of Project: A critical compilation of "Atomic Energy Levels" as derived from the Analyses of Optical Spectra. The tabular data include electron configurations, term designation, J-values, energy levels, term intervals and g-values.

The tables of energy levels are accompanied by "Multiplet Tables" in which related lines are grouped by multiplets. Intensity estimates, excitation potentials, designations, and multiplet numbers are given for individual lines.

Properties and Species: All atomic and ionic spectra of each chemical element are included, provided that atomic structure has been determined from laboratory observations of the individual spectra.

Products Issued: This project was in existence for many years prior to the establishment of NSRDS. It has published a number of tables listed below, as well as miscellaneous articles in press in outside journals.

- (a) NBS Circular 467, Vols. I, II, III, Atomic Energy Levels as Derived From the Analysis of Optical Spectra.
- (b) NBS Circular 488, Sections 1, 2, 3, 4, 5, An Ultraviolet Multiplet Table.
- (c) NBS Technical Note 36, A Multiplet Table of Astrophysical Interest.
- (d) NSRDS-NBS-3, Section 1, Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables, Si II, Si III, Si IV.
- (e) NSRDS-NBS-3, Section 2, Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables, Si I.

A monograph on Yb II, based on unfinished work of W. F. Meggers, is in press.

Status of Work: Manuscript is partially prepared for about 30 additional spectra to be included in this series.

Future Plans: Additional sections of NSRDS-NBS-3 are in demand and will be prepared as soon as possible.

Monographs on Hf I and Yb I, based on unfinished work of W. F. Meggers, are in course of preparation.

Comments: The new series NSRDS-NBS-3 is essentially a revision of "Atomic Energy Levels" Volume I, together with revised Multiplet Tables. It was started in response to many requests for revised data.

The author has been requested to prepare a bibliography giving references to work on the analyses of atomic spectra published since the above volumes appeared in print. This is partly done but needs to be completed with critical evaluation. A bibliography is also requested on rare-earth spectra; this is partly done but needs critical editing.

7. Title: Atomic Transition Probabilities Data Center

Location: Atomic Physics Division, NBS

Principal Investigator: W. L. Wiese

Date Initiated: 1960

Technical Scope: This activity is concerned with the numerical data for atomic transition probabilities, which determine essentially the intensities of spectral lines. The two specific objectives are: (a) the survey of the past and current literature in order to obtain complete bibliographies on these data, and (b) the critical compilation of atomic transition probabilities from all available literature sources for the lightest 20 elements and for selected heavier elements. In selecting the material, particularly the needs of plasma physics, spectroscopy space physics and astrophysics are considered. This project receives its financial support from the Department of Defense, Advanced Research Projects Agency. Close cooperation is maintained with NSRDS and other data centers in related fields.

Properties and Species: Atomic transition probabilities for allowed and forbidden discrete lines of atomic and ionic species.

Products Issued: (1) NBS Monograph 50, "Bibliography on Atomic Transition Probabilities," August 1962, (2) NBS Miscellaneous Publication 278, "Bibliography on Atomic Transition Probabilities," April 22, 1966 (this supersedes NBS Monograph 50), and (3) NSRDS-NBS-4, "Atomic Transition Probabilities, Vol. I, Hydrogen Through Neon" (critical compilation).

Status of Work: By now about 1100 papers have been collected and incorporated into our files. Our cataloging system has been recently converted from a fully manual operation to a semiautomatic storage system. Each pertinent literature reference is punched onto a separate card, so that each of these cards constitute a single entry in our storage system. This new system should greatly speed up the publication of new bibliographies.

The critical evaluation of the data for the second 10 elements from sodium to calcium is being prepared for publication.

Future Plans: The Center expects to start on a critical compilation of atomic transition probabilities for heavier elements sometime during 1968. Also, it expects to issue a new bibliography sometime during next year, since the available literature references have increased now by approximately 25% since the issuance of the last bibliography. It is estimated that the volume containing the critical data for the second 10 elements from sodium to calcium will be in print in the latter part of 1968.

8. Title: Critical Evaluation of Gas Laser Transition Data

Location: Yale University

Principal Investigator: W. R. Bennett, Jr.

Date Initiated: September 1, 1965

Description of Project and Properties Covered and Species Being

Investigated: A continued compilation is made of published gas laser transition data. Reported data are subjected to a number of tests to determine the reliability of transition identification and degree of ambiguity of the assignment. Comparisons of the reported wave-length are made with all possible allowed transitions derived from compilations of critically evaluated atomic energy level data. These comparisons are made with computer techniques to permit listing the identity and number of transitions which fall within the reported or estimated error for the individual laser experiments. A level of certainty in the identification is then determined which depends on the number of possible ambiguities. An overall reliability rating is given to the transition identification which uses both the laser wavelength measurement and alternative methods for the determination of the excited states involved. In addition to the wavelength and transition identification, the criteria by which oscillation was established in the experiment are also examined and given a reliability rating.

For convenience to the users of these data, compilations of related data (with references) which have not been critically evaluated are also listed on a continuous basis. These latter data include optimum gas pressures, gain measurements, power and efficiency measurements and cross section and line width measurements where available.

It is planned eventually to have a continuously-edited printing of the data made available on a periodic basis. However, this periodically revised compilation of results will not become available until the project has completed intermediate stages of the evaluation procedure and formalization of the final printing format. This project receives its financial support from the Department of Defense, Advanced Research Projects Agency.

Status of Work: Work in the last year has been directed toward automating the procedures leading up to the actual evaluation of observed laser wave-lengths in terms of the wave-lengths generated in the catalogues of observed transitions. This approach has resulted in a new generation of programs as well as improvements upon the old programs.

The essence of the approach is to have the computer do the manipulative work of the editing in order to reduce the tedium and improve reliability and expand the range of consideration — as well as make subsequent editing a simple matter. The need for automating and revising the method of approach became obvious after an initial editing of the laser transition data for the noble gases. It was found particularly important to develop a source-oriented reference program. Each laser research paper is given a reference number. Statements are entered regarding the wave-length transition and species assignment made by the author, the type of measurement, the error and the type of error. The catalogue of allowed transitions in that atomic species, and neighboring species of ionization for the same atom, is then searched and the

number and identity of allowed transitions falling within a few integral multiples of the error are printed out. In addition all other laser transition references falling within their own limits of error of the new entry are printed as well. This list is then ordered by nearness to the investigator's wave-length.

Duplication of this process by hand would be next to impossible. The number of ambiguities which have resulted in this compilation is about three times larger than had been anticipated in the beginning of the study and this has emphasized the importance of the additional program modifications. Modification of a number of previous programs was needed for compatibility with the requirements of the new program and a number of improvements have been made in the form of the old output which make the overall procedure much easier and insure greater objectivity in the evaluation. The preliminary form of the new program has been written so that requirements of the later stages could be anticipated while writing the first stages. A sub-routine has now been written which reads the wave-lengths for the transition data that only requires one catalogue consultation within a species in its operation. In addition a prototype program has been written which produces the prescribed number of catalogue transitions nearest the investigator's wave-length. This prototype program is not trivial because of the vast requirements on high speed memory for editing the large number of references typically found within a given atom. The amount of space for each catalogue and the tape read-in time for each catalogue has been reduced by adopting a new abbreviated form. The present abbreviated form has provision for up to 676 levels per species. With this code a transition is labelled by two pairs of letters defining the upper and lower levels. This procedure permits storing the transition identification data with much greater economy than in the previous program. For example, the space required for this output is roughly twice the space required for the energy level data itself. This represents a reduction in the space required for a complete listing by a factor of about twenty over the previous programs. The economy of the present abbreviated listing might in fact warrant the publication of the individual catalogues themselves. (The size of such a complete publication in abbreviated form would be in the order of three times the size of the volumes for the corresponding energy levels.)

Future Plans: It is anticipated that the first installment of the results of the laser evaluation program (primarily devoted to Argon) should be available for publication in the near future. It is planned to continue the present evaluation program next year at about the same level of activity.

Comments: It should be emphasized that the present efforts represent the initial background work for a relatively long-term assignment. It will probably take several years before the distilled effort of this work can be presented in published form for all the atomic and molecular species.

9. Title: Precision X-Ray Measurement and Analysis

Location: X-Ray Laboratory, Physics Department, The Johns Hopkins University, Baltimore, Maryland 21218

Principal Investigator: J. A. Bearden

Date Initiated: June 15, 1965

Description of Project: This project is primarily directed toward precise X-ray spectroscopic measurements, as well as other precision X-ray experiments, especially those bearing on atomic constants.

Properties and Species: This project is mainly concerned with the wavelengths of the stronger X-ray emission lines in the range 0.2 - 10.0 Å, which comprises all but the very soft X-ray spectrum. The project also includes polarization measurements of bremsstrahlung.

Products Issued: The following papers have been published or accepted for publication since April 1, 1966:

- (a) J. A. Bearden, "X-Ray Wavelengths," Rev. Mod. Phys. 39, 78-124 (1967). *
- (b) J. A. Bearden and A. F. Burr, "Re-evaluation of X-Ray Atomic Energy Levels," Rev. Mod. Phys. 39, 125-142 (1967). *
- (c) R. D. Deslattes, H. S. Peiser, J. A. Bearden, and J. S. Thomsen, "Potential Applications of the X-Ray/Crystal Density Method for Comparison of Atomic Weight Values," Metrologia 2, 103-111 (1966).
- (d) J. A. Bearden, J. G. Marzolf, and J. S. Thomsen, "Crystal Diffraction Profiles for Monochromatic Radiation," accepted by Acta Crystallographica, September 1967.
- (e) F. Y. Yap, "Computer Calculations of X-Ray Wavelengths From Double-Crystal Spectrometer Data" (abstract), Bull. Am. Phys. Soc. 11, 388 (1966).
- (f) F. Y. Yap, "Statistical Error Analysis of Wavelength Criteria for X-Ray and y-Ray Spectra" (Doctoral Dissertation, Johns Hopkins University, 1967).
- (g) J. S. Thomsen and F. Y. Yap, "Effect of Statistical Counting Errors on Wavelength Criteria for X-Ray Spectra," accepted by NBS Jour. Res., Sect. A., Phys. and Chem., September 1967 and tentatively scheduled for publication for Feb. 1968.
- (h) J. S. Thomsen, "A Simple Graphical Method for Locating the Peak of a Lorentzian Curve (a Witch)," J. Appl. Phys. 37, 5004 (1966).

* These articles have been reprinted as NSRDS-NBS-14.

- (i) J. S. Thomsen, "Calibration of a Divided Circle, Using Two Diametrically Opposite Pairs of Microscopes" (abstract), Bull. Am. Phys. Soc. 11, 388 (1966).
- (j) R. L. Hickerson, "A Precision X-Ray Target Regulator for ac and dc Filament Power Supplies," (Master's essay, Johns Hopkins University, 1966).
- (k) J. L. Meredith, "A Numerical Method for Unfolding X-Ray Spectra," (Master's essay, Johns Hopkins University, 1967).

Present Status: (a) Four secondary standard reference lines ($Ag K\alpha_1$, $Mo K\alpha_1$, $Cu K\alpha$, and $Cr K\alpha_2$) have been remeasured relative to the primary standard, $W K\alpha_1$. Statistical evaluation and small theoretical corrections should be completed shortly. (b) A study of the effect of statistical counting errors on three possible wavelength criteria (peak, centroid, and median) has been completed. A comprehensive paper has been prepared and accepted for publication in NBS Jour. Res., Sect. A. (c) Work is now well advanced on a ruled grating determination of the conversion factor between the X-ray wavelength scale (\AA^* units) and absolute units. Improved techniques for ruling X-ray gratings have been developed. A precision crystal measurement of the $Al K\alpha_{1,2}$ line has been made, yielding a preliminary value of 8.34032 \AA^* for the centroid of the doublet. Ruled grating measurements of this doublet are now in progress.

Future Plans: (a) Work on items (a) and (c) in the previous section will be completed as rapidly as possible. (b) Additional wavelength measurements will be made in various cases where the need is indicated. In some instances existing data are inaccurate or conflicting. A few wavelength values were found inconsistent with energy levels determined from the rest of the emission line data for certain elements. (Item 7, reference (b)). (c) Bremsstrahlung polarization measurements will be obtained with a gas-target mercury-vapor tube in order to test and to verify the results of Huffman's work (Bull. Am. Phys. Soc. 10, 548 (1965)) over a wider energy range.

Comments: The relatively small effort in X-ray spectroscopy and other precision X-ray experiments within the United States, as contrasted with the renewed interest in this subject in other countries, emphasizes the importance of a continued effort in this field.

10. Title: X-Ray Attenuation Coefficient Information Center

Location: Radiation Theory Section, Radiation Physics Division, NBS

Principal Investigator: J. H. Hubbell

Technical Scope: To generate and periodically update standard reference tables of photon and related electromagnetic cross sections, over the energy range from about 0.1 keV to beyond 10 GeV for use by scientists and engineers.

To evaluate and incorporate into these tables experimental and theoretical cross section data from the literature and to utilize evaluated data from the NBS Photonuclear Data Center.

To calculate and tabulate, where present accuracy is inadequate, electromagnetic cross sections such as photoelectric absorption, Compton scattering, pair (and triplet) production and bremsstrahlung, including polarization effects, radiative corrections, and other refinements needed for consistency with measured data.

To serve as information center and coordinator for photon cross section measurement programs at university, government, and other laboratories.

Properties Covered: Photon (X-ray and gamma-ray) attenuation coefficient (total probability or cross section for interaction of a photon with material) and the cross sections for the most frequent types of interactions: (a) photoelectric absorption, (b) Compton (incoherent) scattering, (c) Rayleigh (coherent) scattering, and (d) creation of electron-position pairs. Derived properties such as the energy absorption and energy transfer coefficients.

Species Being Investigated: Present tabulations cover the energy range 10 keV to 100 MeV for 26 elements from ^{1}H to ^{92}U and for H_2O , NaI and concrete. As theoretical understanding improves and more experimental data are available and evaluated, tabulations will eventually be extended to all elements and to additional substances.

Products Issued: Completion of a program of theoretical calculations related to bremsstrahlung and pair production, resulting in published results on electron and positron polarization, screening effects in elastic electron scattering, and a review article on electron scattering without atomic or nuclear excitation.

H. Olsen and L. C. Maximon, "Polarized electrons and positrons by tagging technique," Physical Review Letters, 13, 112-114 (1964).

J. W. Motz, H. Olsen, and H. W. Koch, "Electron Scattering Without Atomic or Nuclear Excitation," Reviews of Modern Physics, 36, 881-928 (1964).

K. Mork and H. Olsen, "Radiative Corrections, I. High-Energy Bremsstrahlung and Pair Production," Phys. Rev., 140, B1661-1674 (1965).

K. Mork, "Pair Production by Photons on Electrons," Phys. Rev., 160, 1065-1071 (1967).

K. Mork, "Integrations of the Cross Section for Double Compton Scattering and the Radiative Corrections to Compton Scattering," to be published in Phys. Rev.

J. Hubbell and M. J. Berger, "Photon Attenuation and Energy Absorption Coefficients. Tabulations and Discussion," (NBS Report 8681, Sept. 28, 1966) in the Engineering Compendium on Radiation Shielding (International Atomic Energy Agency, Vienna), R. G. Jaeger, Ed. (Springer-Verlag, Berlin, in press).

"Tables of Attenuation and Energy Absorption Coefficients," in Radiation Dosimetry, Vol. 1, Attix, Roesch and Tochilin, Eds. (Academic Press, New York, in press).

Status of Work: Present activities, in addition to answering day-to-day requests for specific photon cross section information (about 400 requests per year), are centered around preparation of an NSRDS report combining the above tables in the Engineering Compendium on Radiation Shielding and in Radiation Dosimetry. Estimated manuscript completion date is Dec. 1, 1967.

Future Plans: Continue revision of tables using new theoretical and experimental data, and to extend energy range of tabulations down to 0.1 keV and up to 100 GeV (BeV), perhaps in collaboration with R. D. Deslattes of the NBS Inorganic Materials Division. Continue to collaborate with a research team under W. H. McMaster at the Lawrence Radiation Laboratory, Livermore, Calif. in revising the DASA-sponsored 1 keV - 1 MeV "Compilation of X-Ray Cross Sections," UCRL-50174 (Sec. II) Jan. 1967, now including 87 elements. Continue to encourage, coordinate, and in some cases support new theoretical calculations as needed to meet the increasing accuracy requirements of attenuation coefficient users.

Comments: Technical areas served by this center include:

- (a) Radiation shielding design (reactors, space vehicle, medical, civil defense).
- (b) Analysis of nuclear physics experiments and of medical X-ray effects.
- (c) Thickness and density gauges.
- (d) Irradiation technology (food preservation; plastics polymerization).
- (e) Electron microprobe analysis (metallurgy).
- (f) Ionosphere prediction (radio propagation).

11. Title: Atomic and Molecular Processes Information Center

Location: Oak Ridge National Laboratory, Oak Ridge, Tennessee

Principal Investigator: C. F. Barnett

Date Initiated: 1964

Technical Scope: The center's activities are concerned with literature search and critical evaluation of both theoretical and experimental data in the fields of heavy particle-heavy particle atomic collision cross sections; particle interactions with quasi-static electric and magnetic fields; and particle penetration in matter. Molecular interactions are considered for those molecules consisting of less than 5-6 atoms. The initial evaluations and compilations are published as review monographs by a commercial publisher.

This project is jointly supported by the Atomic Energy Commission and the National Bureau of Standards.

Products Issued: This project has issued seven annotated bibliographies as internal government reports. A critical monograph, "Ion-Atom Rearrangement Collisions," has been completed and is in the editorial stages of being published by John Wiley & Sons.

Status of Work: Evaluated bibliographical references for 1963-67 consist of approximately 10,000 entries and are now stored in our bibliographical file. The literature search for the years 1950-1962 is 80% complete and when finished in late 1967 will be combined with the present file. The file will then contain 90% of the papers published within our scope of responsibility. The data file consisting of evaluated collision data is in the embryo stage and will be cross linked by computers to the bibliographical file.

Future Plans: References for the years 1950-1962 will be published as a composite annotated bibliography. The second critical review, "Excitation, Ionization and Dissociation by Heavy Particles," will be completed in spring 1968. Plans for two additional monographs are being finalized and work has begun on the third one, "Charge Exchange." The fourth review will be entitled, "Particle Interactions With Quasi-Static Electric and Magnetic Fields." Completion date of these last two reviews will be within the next 18-24 months.

12. Title: Atomic Collision Cross Section Information Center

Location: Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, Colorado

Principal Investigator: L. J. Kieffer

Date Initiated: May 1960

Description of Project: The Information Center collects published reports which contain low energy atomic collision data of interest to plasma physicists and astrophysicists. Current literature is surveyed in order to obtain a complete bibliography of such data, which is then compiled and critically evaluated.

The Information Center was established with partial support from the Department of Defense, Advanced Research Projects Agency. ARPA retains a strong interest in the program and in the output of the Center; it has supported at least a portion of the program of critical review monographs which are being written by leading atomic physicists on the basis of the compilations prepared by the Information Center.

Properties Covered: Low energy electron collision cross sections, photoionization and absorption cross sections, and electron swarm data for atoms and simple molecules.

Products Issued:

- (a) JILA Report No. 30, A Compilation of Critically Evaluated Electron Impact Ionization Cross Section Data for Atoms and Diatomic Molecules.
- (b) JILA Information Center Report No. 3, An English translation of Effective Cross Sections for Collisions of Electrons with Atoms, Atomic Collisions III.
- (c) NBS Miscellaneous Publication 289, Bibliography of Low Energy Electron Collision Cross Section Data.
- (d) JILA Information Center Report No. 4, A Bibliography of Electron Swarm Data.
- (e) "Electron Impact Ionization Cross Section Data for Atoms, Atomic Ions, and Diatomic Molecules: I. Experimental Data," Reviews of Modern Physics, 38, 1 (1966).
- (f) "Electron Impact Excitation of Atoms," Reviews of Modern Physics, January 1968.

Status of Work: Photon and swarm bibliographies are being compiled; a comprehensive data collection for low energy electron collision cross sections is being compiled.

Future Plans: Continue bibliography and data compilation and issue the following: (1) Critical reviews of "Elastic Scattering and Total Cross Section Data," and "Photoionization and Absorption Cross Section Data." (2) Bibliographies of "Electron Swarm Data" and "Photoionization and Absorption Cross Sections." (3) Data compilations of "Electron Collision Cross Section Data" and "Photoionization and Absorption Cross Section Data."

13. Title: A Review of the Effect of Excitation Upon Atomic Collision Cross Sections

Location: General Dynamics, General Atomic Division, John Jay Hopkins Laboratory for Pure and Applied Science, P.O. Box 608, San Diego, California 92112

Principal Investigator: J. William McGowan

Date Initiated: June 6, 1967

Technical Scope: Energy balance in non-equilibrium gaseous systems depends critically upon the reaction and energy transfer cross sections of the excited particles in such systems. Furthermore, it is necessary to know the cross sections for collisions with many kinds of species like electrons, ions, atoms, molecules, and surfaces. The purpose of the present project is to critically review and summarize what information is presently available on the production and destruction of long-lived and metastable excited species.

This project is designed to meet a specific need, that is, a need for summary information on the chemical physics of the excited state. This material finds direct application in the physics of the D and E regions, the polar cap, laboratory plasmas, the chemistry of re-entry shock waves, and a host of problems of special interest to ARPA and other DoD agencies.

Properties and Species: Excitation, de-excitation and energy transfer collisions are being considered for atomic and diatomic ionic and neutral species.

Products Issued: No material is yet ready for publication.

Status of Work: A critical summary of the effect of excitation on ion and electron collisions is presently being prepared.

Future Plans: Following the review of ion and electron collisions affected by excitation, two other topics will be immediately undertaken. They are to be a review of methods of formation of long-lived excited species and a detailed study of the methods of long-lived excited particle detection.

14. Title: Evaluated Infrared Spectra of Organic Compounds of Interest to the Pharmaceutical Field

Location: ASTM Headquarters, 1916 Race St., Philadelphia, Pa. 19103

Principal Investigator: L. E. Kuentzel (to Sept. 1, 1967), Wyandotte, Mich., Mrs. Clara D. Smith, Cranbury, N.J.

Date Initiated: May 1966

Technical Scope: This project is basically concerned with the provision of infrared reference data to be used for comparison purposes by laboratories utilizing infrared spectroscopy for compound analysis and identification. The objective of this activity is the collection, critical evaluation, coding, indexing, and the dissemination of infrared spectral data with emphasis on the field of steroid and pharmaceutical compounds. The spectra to be included in the final collection undergo careful scrutiny and must meet well-defined specifications set to insure that only the best representative spectrum of a given compound will be published in the file. The

project is totally financed by the National Standard Reference Data System under the administration of the National Bureau of Standards.

Properties Covered: Spectral absorption bands; chemical structure; melting point and boiling point; molecular formula.

Status of Work: Over 10,000 spectra have been collected from private and U.S. government laboratories, microfilmed, and are in various stages of evaluation and editing. Of the more than 1500 spectra which have been completely evaluated and edited, there are 500 infrared spectra which meet all specifications and are awaiting final editing for publication. There is an additional group of approximately 200 spectra of good quality which are being held; pending further review and comparison with other spectra, they may or may not be acceptable for inclusion in the file.

Future Plans: Process and evaluate the remaining 5000 spectra on hand for publication.

Comments: The project has been reorganized and since September 15, 1967 has been located at ASTM Headquarters, 1916 Race Street, Philadelphia, Pa., with R. M. Sherwood of the ASTM staff as project administrator. The published evaluated spectra will be made available to the general public in the form of individual data sheets which include the absorption spectrum, basically of a quality satisfying the Class III spectra as designed by the Coblenz Society Specifications (see Analytical Chemistry, Vol. 38, No. 9, August 1966, p27A). It would appear that the long range needs of this field are such that Class II spectra (Coblenz Society Specifications) will be of great value to the field in the not-too-distant future. In view of the improved instruments available to this field, the Class II spectra will be considered as a fruitful area of development for this and related projects.

15. Title: Infrared Reference Spectra Specifications

Location: The Coblenz Society, Inc., 761 Main Avenue, Norwalk, Connecticut 06851

Principal Investigator: Nelson Fuson, President, The Coblenz Society, 1966-68, Box 8, Fisk University, Nashville, Tennessee 37203

Date Initiated: June 3, 1965

Description of Project: To develop a written procedure for evaluation of infrared spectra, and to consider the need, the sources, and the uses of a relatively small collection of highest quality infrared spectra.

Properties Covered: Infrared spectra.

Products Issued: "Specifications for Evaluation of Infrared Reference Spectra," by the Coblenz Society Board of Managers, Anal. Chem. 38, 27A-38A (1966).

Status of Work: The Board of Managers of the Coblenz Society met four times during 1965 and 1966 to work out the specifications for eval-

ation of infrared reference data. These specifications were further considered at subsequent meetings of the Board. The publication of these specifications developed during these intensive sessions is identified above.

Future Plans: The Coblenz Society Board of Managers asked Dr. R. Norman Jones to chair a Sub-Committee on Evaluation of Reference Spectra whose responsibility is to evaluate criticisms of the specifications we drew up and to bring recommendations to the Board. As a result of a call from this sub-committee the Coblenz Board of Managers met on Friday, December 1, 1967, in Chicago, Illinois, to consider Class II specifications and to discuss possible more stringent specifications prior to the international consideration of spectral standards by IUPAC.

Comments: Following projected meetings of the Coblenz Society Board of Managers, revisions of the specifications, and additional comments will be forth-coming.

16. Title: Microwave Spectral Tables

Location: Atomic Physics Division, NBS

Principal Investigators: David R. Lide, Jr.; Wm. H. Kirchhoff

Date Initiated: January 1967

Description of Project: The objective of this project is to provide a continuing data center for the collection, critical evaluation, and dissemination of data on the microwave spectra of gases. The input comes from published literature and from private communication with scientists working in the field of microwave spectroscopy. Microwave frequencies are evaluated with regard to accuracy and correctness of interpretation. Tabulations of frequency and related data will be published at regular intervals as supplements to the previous NBS tabulation of microwave data (Monograph 70). The data are required by microwave research workers and by others concerned with the use of microwave spectra for purposes of chemical analysis.

Properties Covered: The tabulation will include the frequencies of transitions between the energy levels of molecules falling in the microwave and millimeter regions, typically from 300 MHz to 300,000 MHz. The molecular spectra occurring in this region are generally associated with the rotational energy levels of molecules although in special cases transitions between vibrational or electronic energy levels also fall in the microwave region. There is no limit on the species being investigated but the nature of the experimental techniques as well as the interaction of the molecules with the microwave radiation requires that the species be studied in the gas phase and have a permanent dipole moment.

Products Issued: This project originated in the Radio Standards Physics Division, NBS Boulder, before being transferred to the Atomic

Physics Division, NBS Washington. Publications issued by this project from the Radio Standards Physics Division are: "Microwave Spectral Tables, Diatomic Molecules," NBS Monograph 70, Vol. I, and "Microwave Spectral Tables, Line Strengths of Asymmetric Rotors," NBS Monograph 70, Vol. II. Now in press are "Polyatomic Molecules With Internal Rotation," NBS Monograph 70, Vol. III, "Polyatomic Molecules Without Internal Rotation," NBS Monograph 70, Vol. IV, and "Spectral Line Listing," NBS Monograph 70, Vol. V.

Status of Work: A collection of reprints covering the published microwave work from 1960 to 1966 has been almost completely assembled. In addition several meetings with interested representatives from industry, universities, and Government agencies have been held for the purpose of discussing the possibility of exchange of non-critical, unpublished microwave spectra with NBS acting as a general clearinghouse. Because the published microwave spectra represent only a partial presentation of the microwave spectrum of the species studied (usually only those transitions which have been assigned to specific energy level differences), a table of this sort is not very useful for certain problems in chemical analysis. The exchange would be by means of media compatible with computers (punched cards or tapes). A format for presenting this information has been agreed upon and a few laboratories are carrying out such an exchange to test the feasibility of this type of program.

Future Plans: With the assistance of several members of the Infrared and Microwave Spectroscopy Section, evaluation of the collected papers will begin in the near future and the pertinent information will be transferred to punched cards for the purpose of computerized sorting and eventual printing. The first supplement will cover material published from 1960, the cut-off date of Monograph 70, to 1966.

Comments: In order to refer in a computer to the spectrum of a specific compound, it is necessary to assign a reference number to each compound studied and it would be desirable if this number would have some significance outside the framework of the microwave spectral tables. The American Chemical Society, within the offices of the Chemical Abstracts Services, is preparing a registry of chemical compounds, and to use this registry number in the microwave spectral tables would be most useful.

17. Title: Compendium of ab initio Calculations of Molecular Energies and Properties

Location: Physical Chemistry Division, NBS

Principal Investigator: Morris Krauss

Description of Project: The number of ab initio molecular electronic calculations has increased dramatically in the last few years. Both the practitioners and other interested students of the results of the calculations have found it increasingly difficult to determine the present

status of these calculations. This compendium references the work from 1960 to the present and abstracts from the mass of data the best values for several observable properties including the total energy, dissociation energy, electron affinity, spectroscopic constants, electric moments, field gradients, polarizabilities, and magnetic constants. In order to provide an insight into molecular electronic structure tables of orbital energies are also included.

These tables are meant to direct attention to the successes and failures of the calculations by compiling a large percentage of the best results in a reasonably compact form. Its usefulness will be limited in time by rapid advance in the field.

This work was supported by the Advanced Research Projects Agency.

Products Issued: NBS Technical Note 438, Compendium of ab initio Calculations of Molecular Energies and Properties, by M. Krauss.

Status of Work: Completed.

VI. SOLID STATE

Although quantitative data on the properties of solid substances are recognized to be of considerable importance for science and technology, only a very small program has been developed under the auspices of the National Standard Reference Data System. This has been the result of an administrative decision to concentrate available resources on other types of data rather than to spread out thinly to attempt to cover more subjects. For this reason the number of projects and the number of products are small.

There has been one publication from projects supported by the Office of Standard Reference Data in this area since the previous Status Report. This is Superconductive Materials and Some of Their Properties, by B. W. Roberts, NBS Technical Note 408, September 1966. This is a non-critical compilation of data on the structure, crystallography and other properties of superconductive materials.

For a considerable time the principal emphasis of the program of the Office of Standard Reference Data on solid state properties has been placed on publication of the third edition of Crystal Data Determinative Tables. Several of the projects support this aim, as do other activities which do not receive support from the Office of Standard Reference Data. This monumental task is now approaching completion. When completed the tables will appear as a National Bureau of Standards publication in the National Standard Reference Data series.

The revision of Crystal Data Determinative Tables has been the major mission of the Crystal Data Center of the Institute for Materials Research of the National Bureau of Standards. The tables will contain crystallographic data abstracted from the scientific literature and a bibliography for the use of crystallographers, mineralogists, chemists, and physicists. The data to be included are axial lengths and angles of the unit cell, space groups, number of molecules or formula weights per cell, both the measured densities and those computed from X-ray data, habits, cleavages, twinnings, colors, refractive indices, and melting points. Although detailed structural information such as that in Structure Reports will not be given, the tables will provide pertinent references to structural studies. All data will be carefully referenced to the original literature.

The first edition of Crystal Data, which was published in 1954 by the Geological Society of America as Memoir 60, contained about 6000 entries including data current to January 1, 1952. In 1963 the second edition appeared as Monograph Number 5 of the American Crystallographic Association. This edition had around 13,000 entries current to January 1, 1961. The approximately 30,000 entries of the third edition will be current to January 1, 1967.

The tables are being prepared under the general supervision of the

Crystallography Section of the NBS Institute for Materials Research.
The scientific staff for this work are:

Chief Editor — J.D.H. Donnay, The Johns Hopkins University,
Guest Worker at NBS
Assistant Editor — H. M. Ondik, NBS
Organic Editor — O. Kennard, Cambridge University
Inorganic Editors — H. M. Ondik, NBS; G. Wolten, Aerospace Corp.
Mineral Editor — M. Mrose, U.S. Geological Survey
Intermetallic Editors — S. Samson, California Institute of Technology; M. Mueller, Argonne National Laboratory; Q. Johnson, Lawrence Radiation Laboratory; and E. Ryba, Pennsylvania State University
Protein Editor — M. V. King, Massachusetts General Hospital

The third edition will be produced by tape-controlled photocomposition. The editing of the tape will be done by computer.

The text and data are being keyboarded into punched paper tape, partly from the previous edition and partly from sheets on which new information has been recorded. One-fourth to one-third of the information is new. Keyboarded data are processed through a phototypesetting machine which produces a film positive. The film positive is proofread and corrections marked.

All data from these tapes are transcribed automatically on magnetic tape by a special transcriber. The magnetic tapes are fed into a general-purpose computer, which first inserts the corrections and then performs a variety of editing tasks. The information is arranged into the order in which it is to appear in print. Some arithmetic checks are applied to the numerical information. Literature references are compared with a computer-stored list of standard abbreviations of journal titles. The computer then prepares two alphabetical indexes — one by chemical formula, one by chemical compound name. These are put automatically into the arrangement in which they are to be printed.

Finally, the computer deletes certain keypunched signals which are not wanted in print and breaks the copy into lines of proper length, inserting spaces between paragraphs, breaking into pages, inserting page headings, and page numbers. The output of the computer is recorded on magnetic tape which is converted to a 15-level paper tape. The latter drives a photocomposition unit operated by the Government Printing Office.

The second edition took three years to produce, largely because of the time needed to make up the indexes. Production by computer should save time and avoid errors in routine indexing through its automatic checking features. Another great advantage is expected to be the ease of inserting future corrections and additions; completely up-to-date information will always be available on tape and can be printed more frequently with less effort.

Detailed descriptions of the various projects on solid state properties

follow. The first three projects are directly concerned with the Crystal Data Determinative Tables.

1. Title: Crystal Data

Location: The Johns Hopkins University, Baltimore, Md. 21218, and NBS

Principal Investigators: J.D.H. Donnay (JHU) and Helen Ondik (NBS)

Date Initiated: 1964

Technical Scope: Collecting and, whenever possible, evaluating crystallographic data published from 1912 on.

Properties Covered: The data comprise: cell dimensions, obtained by X-ray diffraction methods, space-group symmetry, cell contents, structural information, density (measured), density (calculated), name of compounds, chemical formula, literature reference, remarks. Under remarks are given some auxiliary physical properties, useful for determinative purposes, such as: optical properties, melting point, color, crystal habit, transformation point. The data are classified according to crystal systems. To each system the compounds are listed according to axial ratios.

Products Issued: Two editions (1954 and 1963) were issued prior to the beginning of the present project, which is carried on under joint sponsorship of the American Crystallographic Association and NBS.

Status of Work: The data are all on paper tape, most also on magnetic tape. The completed third edition is expected to exceed 30,000 entries, although a large number of entries have been deleted from the second edition. The second edition numbered about 13,000 entries. The computer programs are about 90% complete. They are being written for purposes of checking, sorting, retrieving, and operating of the typesetting machine.

Future Plans: The third edition will, of necessity, comprise two volumes: The first volume will be devoted to Organic Compounds, including Proteins in an Appendix. The second volume will deal with all other substances.

It is planned to issue Vol. 1 by mid-1968. Vol. 2 should then follow shortly afterwards.

Comments: Monograph No. 6 of the American Crystallographic Association is in press at this time. It is the last publication supported by ACA and represents the second part of the second edition. It covers about 200 pages. It is authored by W. Nowacki (University of Berne, Switzerland). It lists all the compounds that crystallize in any given space group. In the future such information will be made available as computer output, thanks to our programs.

2. Title: Compilation and Critical Evaluation of X-Ray Data on Crystalline Organic Compounds

Location: University Chemical Laboratory, University of Cambridge, Cambridge, England

Principal Investigator: Olga Kennard

Date Initiated: July 1963

Description of Project: This project is part of the work on the revision of the book Crystal Data. In this section data on crystal properties of organic materials will be compiled, evaluated and put into a form suitable for machine handling. The product will be reference data of wide use in identifying and understanding the properties of organic crystals. Data will be compiled and evaluated and stored on tapes in a form suitable for editing and printing by machine.

Properties and Species: See project description above.

Products Issued: See project description above.

Status of Work: The Cambridge project takes full responsibility for: (1) the scanning of the literature for all compounds, (2) abstracting and updating of data relevant to carbon containing compounds, excluding proteins, and (3) abstracting of papers on inorganic compounds during 1965/1966.

Literature references are traced through the "Bulletin Signaletique," the abstracting journal published by the Centre National de la Recherche Scientifique, Paris, and periodically cross-checked against the relevant issues of the Chemical Abstracts. Should the paper refer to a compound already in the Crystal Data files a careful comparison is made and the old entry updated wherever possible.

A number of abstracts are received directly from the National Data Committees of the International Union of Crystallography. In particular over 300 abstracts are received from the U.S.S.R., annually. These are edited and transferred to coding sheets. All coded sheets are sent to the National Bureau of Standards in Washington.

During 1967 every effort was made to ensure complete coverage for the years 1960-1966 including preliminary notes, dissertations, conference reports, etc., and considerable time was spent in checking for possible omissions.

All entries for the organic (carbon containing) volume, which will contain data from the literature published prior to January 1, 1967, have been completed and dispatched to NBS.

Future Plans: Because of the increasing rate of publications with a doubling time of about three years, it is essential to continue data

compilation without a break. We plan, therefore, to continue scanning and abstracting of the literature for the years 1967/1968. We plan also to supply about two thirds of the abstracts, those relating to compounds with established structure, in form of punched cards instead of written abstracts. These cards will be computer processed so that part of the checking and mathematical transformations will be carried out in Cambridge. We hope, thereby, to reduce the work of the staff at the National Bureau of Standards, when transferring data from the abstracts to the computer. We also plan to collaborate with the Office of Standard Reference Data on experiments of using these cards for the direct production of Crystal Data.

During 1968 we anticipate to:

- (1) Publish the third edition of the organic section of Crystal Data.
- (2) Provide the Editors associated with the National Bureau of Standards with a full set of papers on the relevant literature of single crystals published during 1967/1968.
- (3) Prepare abstracts and punched data cards for all carbon containing substances — excluding proteins.
- (4) To update and correct the previous edition of Crystal Data.

Comments: Crystal Data is probably the largest computer produced critical data compilation. It was undertaken in part as a pilot project on the feasibility of this approach to scientific publications. The results will have to be evaluated during the coming years. When the book becomes available on magnetic tape it will be possible to list the entries in different ways, prepare more meaningful indexes, compare multiple data on the same substance and develop search procedures for locating particular items of information.

With the increasing power of X-ray techniques, structural information will become available on a rapidly increasing number of compounds. Computer based structural libraries are already being prepared and these will have to be linked closely with Crystal Data. Consideration should also be given to computerized methods of preparing illustrations of compounds and of other means of presenting the results of diffraction analyses to scientists. There is also a possibility that in the future Crystal Data will become a more efficient depository than primary journals of certain types of numerical data, and this possibility should, perhaps, be investigated.

3. Title: Single Crystal Data Correlation

Location: Materials Research Laboratory, The Pennsylvania State University, University Park, Pennsylvania 16801

Principal Investigator: Gerald G. Johnson, Jr.

Date Initiated: March 15, 1967

Technical Scope: This activity is producing computer programs to ascertain the validity (both accuracy and consistency) of the input Linofilm keyboarded entries of the forthcoming edition of Crystal Data. This data is being checked with programs written especially for this purpose using crystallographic theory. The Takada and Donnay cell reduction program is also being used to give a further refinement of the data.

Properties Covered: This work covers those crystallographic properties such as unit cell parameters, space group, density and references which are reported in Crystal Data.

Products Issued: None

Status of Work: The programs developed at Penn State are in the final stages of testing while the Takada and Donnay program has been well tested. Data processing of the input data will be initiated upon receipt of the Linofilm magnetic tape from the National Bureau of Standards.

Future Plans: All crystallographic data in the forthcoming publication of Crystal Data will be processed using these programs. This should result in the publication of this reference within the year. This conversion and checking of the content of Crystal Data will result in a BCD magnetic tape which offers very large possibilities for information retrieval systems.

Comments: The application of self-consistent theory to check the keyboarding of data for publication has proven to be quite successful and should be considered whenever possible, for future publications. The Linofilm-computer knowledge gained should be of value to other computer-oriented groups seeking to use Linofilm input for reference book production with type-set quality.

4. Title: Alloy Data Center

Location: Alloy Physics Section, Metallurgy Division, NBS

Principal Investigator: Dr. G. C. Carter, Project Leader, and
Dr. L. H. Bennett, Chief, Alloy Physics Section

Date Initiated: April 1966

Technical Scope: Recent developments in alloy theory together with modern experimental methods have suggested interrelationships between the properties listed below. It is therefore our goal to stimulate cooperation and coordination among other existing data centers specializing in a few of the listed properties. A system has been developed such that documents concerning a property of a certain alloy, but directly giving valuable information on some other properties of that material, are

properly recalled when needed. Such a tool is necessary to help make complementary data consistent with one another. A file of published alloy data compilations and other books containing smaller tables is being maintained to serve us in our task of guiding and of reviewing certain of the other data compilations before final publication.

In addition there are two major fields of alloy data in which we are directly immersed:

- (1) NMR Data. This includes Knight shifts, also called "metallic shifts."
- (2) Soft X-Ray Data. The parameters obtained here bear directly on energy bands (category 5).

Properties Covered: The center deals with properties grouped in the following nine categories: (1) electronic transport properties, (2) magnetic properties, (3) mechanical properties, e.g., densities, internal structures, acoustical properties, (4) nuclear magnetic resonance (abbreviated NMR) and other resonance properties, (5) Fermi surface and band structure determinations, (6) electromagnetic radiation, excluding the region of "soft X-rays," (7) properties of superconducting materials, (8) thermodynamic properties, and (9) soft X-ray spectroscopy (abbreviated SXS).

In total, over one hundred properties are of interest and are indexed when encountered in the systematic search for the two properties mentioned.

Species: The materials of interest include all metals, binary alloys, and some higher order alloys.

Products Issued: None.

Status of Work: In August 1967 the system was converted to a more flexible system which satisfies our requirements for data reduction. This includes a method of handling errata and other forms of error indications found in the literature. The move was done entirely with use of the UNIVAC 1108 computer, using COBOL as programming language. The main portion of the file contains the SXS material which is completely up-to-date, and the NMR file of which the Knight shift related papers are now entered. Specific search programs have recently been written; a general update and correct program is used for file maintenance and generation of our indexes by author, reference number, and material (alphabetically by chemical symbol).

Evaluation of Knight shifts has recently been started after a final systematic effort of literature searching in abstract journals. The most productive source of documents appeared to be secondary references and articles obtained by scientists in the Alloy Physics Section doing active research in their field of competence. For file maintenance Current Contents is also used. Other specific efforts in literature searching and indexing are described under Comments.

Future Plans: (1) The SXS group plans to prepare a table of soft X-ray spectra, (2) the NMR group will complete a table of Knight shifts in metals and alloys, both solid and liquid, and other materials with metallic properties, and (3) the annotated book file mentioned under Technical Scope will be recategorized and a more careful definition of "data compilation" and "reference book" will be used.

Note: The system has been set up in such a manner that annotated bibliographies in specific experimental fields can be generated from the created alloy data file. (EPR, Electron Paramagnetic Resonance is an example). Other areas of future interest include neutron diffraction and positron annihilation.

Comments: A major part of the fiscal year 1967 literature search was spent on a search for outside automated documentation services. It was hoped that such existing bibliographical services could give the initial base of documents for the new data center which needed such a wide scope of material. The American Society for Metals Information Service proved to be unable to provide the type of bibliographic service needed. No systems provide complete service, however the following give useful results.

- (a) A.S.C.A., the automatic citation index of the Institute for Scientific Information. This prompt service represents a valuable aid for current awareness.
- (b) The D.D.C. automated services. We received a good retrieval covering Technical Reports.

5. Title: Superconductive Materials Data Center

Location: General Electric Research and Development Center, P.O. Box 8, Schenectady, New York 12301

Principal Investigator: B. W. Roberts

Date Initiated: 1965

Technical Scope: To collect, collate, and disseminate information on superconductive materials and to evolve standard values of important parameters for these materials.

Properties Covered: Data tabulated on superconductive materials: Critical temperatures; critical magnetic fields; crystallographic description; source of data; critical magnetic fields of high field superconductors; presence of thermodynamic parameter data is noted; data on non-superconductors when specifically studied.

Products Issued: Superconductive Materials and Some of Their Properties, by B. W. Roberts, NBS Technical Note 408, September 1966.

Condensed presentations in the Handbook of Chemistry and Physics (Chemical Rubber Co.) and the American Institute of Physics Handbook.

Status of Work: A supplement is in preparation. References to the literature are being accumulated.

Future Plans: A second NBS Technical Note is planned for mid-1968.

Comments: Individual queries are answered; periodic reports of new data made available; periodic summations of all known data on superconductive materials and materials tested for superconductivity.

6. Title: Diffusion in Metals and Alloys

Location: NBS

Principal Investigator: J. R. Manning

Date Initiated: 1963

Technical Scope: There are two main types of diffusion experiments: (1) tracer diffusion experiments, in which a very thin layer of radioactive tracer atoms diffuses into a homogeneous crystal, and (2) chemical interdiffusion experiments, in which atoms from bulk specimens in contact intermingle. Data from both types of experiments will be analyzed. This work is being done in conjunction with other theoretical and experimental projects designed to relate tracer and interdiffusion measurements to each other and to the atom jump frequencies.

Properties and Species: Diffusion coefficients and activation energies for diffusion in pure metals and binary alloys.

Products Issued: No product issued to date. Future products will be tables of data of diffusion coefficients and activation energies with discussions of results for individual systems.

Status of Work: Literature search has been completed, and classification and critical evaluation of extracted data are underway.

Future Plans: This is a continuing project, and the data and bibliography will be maintained on a current basis. Work on critical evaluation will be emphasized in the coming year.

7. Title: Binary Oxide Systems

Location: A-225, Materials Building, NBS

Principal Investigator: R. S. Roth

Date Initiated: Fiscal year 1965

Technical Scope: The primary purpose of this project is to critically analyze published data concerning the chemical reactions in binary oxide systems, with the end view of preparing composite phase equilibria diagrams for each system.

Properties and Species: This project covers all elements whose oxides are solids at room temperature and the binary systems involved between any two of these oxides. Properties covered include chemical compounds phase transitions, melting points, etc., necessary to construct phase diagrams, as well as unit cell dimensions, etc. necessary to identify the phases present in the system.

Products Issued: None.

Status of Work: All the old literature up to 1946 has been examined for pertinent data and many copies of the pertinent papers have been indexed and filed.

Future Plans: This project has been terminated.

8. Title: Electrical Resistivity of Metals at Low Temperatures

Location: Cryogenic Data Center, Cryogenics Division, Institute for Materials Research, NBS, Boulder, Colorado

Principal Investigators: L. A. Hall and H. M. Roder

Date Initiated: August 1966

Technical Scope: In the initial phase we are concerned with a non-critical collection of the electrical resistivity data available in the literature. The results are presented graphically and as an annotated bibliography. The product will be of immediate use to the designer; it is also the survey requisite for subsequent critical compilation.

Properties Covered: Electrical resistivity, sample preparation — purity, crystal structure.

Species: Aluminum, beryllium, cobalt, copper, gold, indium, iron, lead, magnesium, molybdenum, nickel, niobium, platinum, silver, tantalum, tin. Others are planned.

Products Issued: None.

Status of Work: An NBS Technical Note, Electrical Resistivity of 16 Pure Metals at Low Temperatures, by L. A. Hall, presently is in press.

Future Plans: Survey is continuing for the following metals: cadmium, chromium, manganese, titanium, tungsten, vanadium, zinc, and zirconium. The work may lead to a survey of the resistivities of alloys — of importance in practical applications. Its logical conclusion is the

critical evaluation of electrical resistivity for pure metals in terms of intrinsic and residual contributions.

Comments: The compilation program is conducted in close liaison with those experimental groups in the division that are engaged in measuring electrical resistivity at cryogenic temperatures.

VII. THERMODYNAMIC AND TRANSPORT PROPERTIES

Thermodynamic and Transport Properties is one of the two major areas of emphasis in the program of the Office of Standard Reference Data. Data compilation and evaluation activities in this area are of broad importance to many technical agencies. Closely allied to the program sponsored directly by the Office of Standard Reference Data are several types of data compilation activities: (1) There is the type of program sponsored by other agencies for which the Office of Standard Reference Data serves as program manager, (2) the program sponsored independently, but which cooperates closely with the Office of Standard Reference Data, and (3) the integrated data program of a research organization among whose activities is included a project supported by the Office of Standard Reference Data. Examples of the first kind are a project on electrolytes in solution at the National Bureau of Standards, sponsored by NASA, and a project on phase diagrams of metals and alloys at IITRI, sponsored by AEC, NASA, and USAF. Examples of the second kind are a diffusion program at the University of Maryland sponsored by NASA and projects at the Cryogenic Data Center of the National Bureau of Standards, Boulder Laboratories, sponsored by NASA and NBS. Examples of the third kind are projects of the Thermophysical Properties Research Center at Purdue University, the Thermodynamics Research Center at Texas A&M, and the Molten Salts Data Center at Rensselaer Polytechnic Institute. Other more loosely coordinated activities on data compilation and evaluation in the area of Thermodynamic and Transport Properties are listed elsewhere in this status report.

Several of the programs have reached sufficient maturity to have produced results. Available publications in the NSRDS-NBS series are:

High Temperature Properties and Decomposition of Inorganic Salts, Part 1, Sulfates, by K. H. Stern and F. L. Weise, NSRDS-NBS-7, October 1966.

Thermal Conductivity of Selected Materials, by R. W. Powell, C. Y. Ho, and P. E. Liley, NSRDS-NBS-8, November 1966.

Another available publication is:

Selected Values of Chemical Thermodynamic Properties, Part 3, Tables for the First Thirty-Four Elements in the Standard Order of Arrangement, by D. D. Wagman, W. H. Evans, V. B. Parker, I. Halow, S. M. Bailey, and R. H. Schumm, NBS Technical Note 270-3, January 1968.

This supersedes NBS Technical Notes 270-1 and 270-2 and is another in a series of publications containing material prepared as a revision of the tables of Series I of National Bureau of Standards Circular 500, Selected Values of Chemical Thermodynamic Properties, by F. D. Rossini, D. D. Wagman, W. H. Evans, S. Levine, and I. Jaffe. When revision of the tables has been completed, a comprehensive version will be issued as part of the NSRDS-NBS series.

In addition to these NSRDS publications, some publications from closely related projects can be mentioned, specifically:

The Viscosity and Thermal Conductivity Coefficients of Dilute Argon Between 90 - 2000 °K, by H.J.M. Hanley, NBS Technical Note 333, March 1966.

Comparison of the Lennard-Jones, Exp: 6 and Kihara Potential Functions Using Viscosity Data of Dilute Argon, by H.J.M. Hanley, J. Chem. Phys. 44, 4219 (1966).

Dilute Nitrogen and Oxygen, by G. E. Childs and H.J.M. Hanley, NBS Technical Note 350, October 1966.

The Viscosity and Thermal Conductivity Coefficients of Dilute Neon, Krypton, and Xenon, by H.J.M. Hanley and G. E. Childs, NBS Technical Note 352, March 1967.

Mention should also be made of the loose-leaf sheets in the Thermodynamics Research Center Data Project and the American Petroleum Institute Research Project 44 series prepared periodically by the Thermodynamics Research Center of Texas A&M University. Other publications less concerned with data evaluation are listed in the detailed reports of the data centers.

There are also several reports in press:

Molten Salts: Electrical Conductance, Density, and Viscosity Data, by G. J. Janz, F. W. Dampier, and P. K. Lorenz, NSRDS-NBS-15.

Thermal Conductivity of Selected Materials, Part 2, by C. Y. Ho, R. W. Powell, and P. E. Liley, NSRDS-NBS-16

Critical Analysis of the Heat Capacity Data of the Literature and Evaluation of Thermodynamic Properties of Copper, Silver, and Gold From 0 to 300 °K, by G. T. Furukawa, W. G. Saba, and M. L. Reilly, NSRDS-NBS-18.

Thermodynamic Properties of Ammonia as an Ideal Gas, by L. Haar, NSRDS-NBS-19.

The last named will also appear in the Journal of Research of the National Bureau of Standards.

Molten Salt EMF Formation Cells, by Chr. G. M. Dijkhuis, Ria Dijkhuis, and G. J. Janz, Chem. Rev., in press.

Results from some of the compilation activities on one project will appear in Heats of Solution of Aluminum, Copper, and Silicon, by F. Woolley and J. F. Elliott, Trans. Metallurgical Soc. AIME, in press.

The following reports have been received and are undergoing review prior to publication:

"Thermodynamic Properties of Pure Aliphatic Alcohols, Part I, General Introduction, Bibliography, and Properties of Eight Normal and Branched Alkanols C_1 to C_8 ," by B. J. Zwolinski and R. C. Wilhoit.

"Phase Behavior in Binary and Multicomponent Systems at Elevated Temperature: The n-Pentane System," by B. H. Sage.

"Phase Behavior in Binary and Multicomponent Systems at Elevated Temperatures: The Methane-n-Pentane System," by B. H. Sage.

Detailed descriptions of each individual project follow.

1. Title: Chemical Thermodynamic Data Project

Location: Thermochemistry Section, NBS

Principal Investigators: D. D. Wagman and W. H. Evans

Date Initiated: 1940

Technical Scope: The principal task is the preparation and periodic revision of the tables of Selected Values of Chemical Thermodynamic Properties. To accomplish this requires the locating and collection of all pertinent thermodynamic data and the systematic critical evaluation of the total available mass of data. A byproduct of this effort is an index to the published thermodynamic data for inorganic compounds prepared for the annual IUPAC Bulletin of Thermodynamics and Thermochemistry. This index summarizes annually the published chemical thermodynamic information with respect to compounds and properties measured, with the appropriate bibliographic citation. Although the project is not basically a data information center, the extensive files of data are used to answer numerous specific inquiries.

Properties and Species: The properties being evaluated include the enthalpy and Gibbs (free) energy of formation, and the entropy, heat capacity, and heat content of all chemical substances, and well-defined mixtures of these, for which data are available.

Products Issued: Selected Values of Chemical Thermodynamic Properties, Part 3: Tables for the First Thirty-Four Elements in the Standard Order of Arrangement, by D. D. Wagman, W. H. Evans, V. B. Parker, I. Halow, S. M. Bailey, and R. H. Schumm, NBS Technical Note 270-3, January 1968.

The 1967 Annual IUPAC Bulletin of Thermodynamics and Thermochemistry which includes the index to the thermodynamic data for inorganic compounds published during 1966, has been published.

Status of Work: Work is continuing on the revision of NBS Circular 500; sections as completed are appearing as NBS Technical Note 270, and will be combined into an annotated volume when the revision is completed. The 1967 index in the IUPAC Bulletin is being prepared. During the year the application of computer methods to the preparation of the index has been extensively explored; we expect to prepare the final copy for the 1967 index, including all sorting and filing procedures, by machine.

Future Plans: The revision of Circular 500 will continue; it may be completed by the end of 1968. At that time the discussion of the data will be prepared; the cumulated tables, the discussion, and the bibliography will be issued as one volume. We plan to resume work on the evaluation of data on heats, temperatures, and entropies of transition, fusion and vaporization of inorganic compounds as soon as the compilation of heat of formation data is completed.

2. Title: Thermodynamics Research Center Data Project (formerly Manufacturing Chemists Association Research Project)

Location: Department of Chemistry, Texas A&M University, College Station, Texas 77843

Principal Investigators: Bruno J. Zwolinski; R. C. Wilhoit, Associate Director; and A. S. Rodgers, Assistant Director

Date Initiated: December 1, 1954

Technical Scope: The Thermodynamics Research Center Data Project (formerly the Manufacturing Chemists Association Research Project) is one of the few academic critical data groups in the world which in a very comprehensive manner produces scientific data on a large number of diversified yet related sets of property values such as P-V-T, physical, thermochemical, thermodynamic, and spectral properties of chemical compounds of interest to the chemical industry.

The staff of the Thermodynamics Research Center searches the chemical literature of the world and locates all documents which contain pertinent physical and thermodynamic data. These data are extracted and collected. The files are reviewed periodically and when sufficient data of a given type have been collected the "best values" are critically selected and a data sheet containing these new or revised data is prepared. Methods of predicting and correlating properties are also developed and are used to fill in gaps where reliable experimental data are not available. A priority list of some 100 organic compounds selected on the basis of tonnage sales in the U.S.A. serves as a guide in these studies.

Properties and Species: Currently the Thermodynamics Research Center Data Project is concerned with pure substances and not mixtures. The properties investigated include P-V-T, physical, thermochemical, thermodynamic, and spectral. These properties are critically selected and

arranged in a convenient form for ready use, covering, in due course, all chemical compounds of interest and importance to chemical technology in the United States. The present emphasis, however, is on organic compounds other than hydrocarbons.

Loose-leaf data sheets are issued semiannually.

The spectral data which are published are contributed by various educational, governmental, and industrial laboratories which are equipped to obtain reliable measurements. These spectra are carefully screened and only high quality spectra on carefully purified compounds are used. The types of spectral data sheets issued include infrared, ultraviolet, Raman, mass, and nuclear magnetic resonance.

Products Issued: Loose-leaf data sheets prepared by the Thermodynamics Research Center Data Project represent a complete and self-consistent set of tables and catalogs of critically selected numerical and spectral data on chemical compounds. These tables and catalogs cover certain inorganic and organic substances of importance to science and technology with the exception of the hydrocarbons and certain related compounds covered by the American Petroleum Institute Research Project 44. There is no duplication or overlapping in the scientific information found in the tables and catalogs of the Thermodynamics Research Center Data Project and of the American Petroleum Institute Research Project 44. These tables and catalogs of critically selected "best values" and of quality spectra are maintained substantially up-to-date by revision at appropriate intervals. Each data sheet carries the date of preparation or revision of the information published. In addition a sheet of "Specific References" is issued for each Table of Thermodynamic and Physical Properties. These Specific References furnish a complete bibliography for each of the properties listed on the table. Those references which are considered in the final selection are identified by means of boldface type. For the past two years the Center has prepared a series of "Technical Notes" which give additional details concerning the selection of data for each table issued during this period. These are written in the form of brief informal notes, and copies may be obtained by writing to the Director.

The scientific loose-leaf data sheets of the Thermodynamics Research Center fall into the following six categories:

- (a) Tables of selected values of physical and thermodynamic properties of chemical compounds.
- (b) Catalog of selected infrared spectral data.
- (c) Catalog of selected ultraviolet spectral data.
- (d) Catalog of selected Raman spectral data.
- (e) Catalog of selected mass spectral data.
- (f) Catalog of selected nuclear magnetic resonance spectral data.

Supplements of new and revised sheets in the six categories are scheduled for issuance twice each year, June 30th and December 31st. Category (a) is issued as scheduled; the issuance of sheets of spectral data may vary from none to two sets per year, depending on the availability of satisfactory data.

The Thermodynamics Research Center also issues several Reports of Investigation each year which describe the results of research work carried out by the staff of the Center, and other information of interest to the users of thermodynamic data. Many of these are also published in the scientific literature.

Finally, the Center prepares special detailed reports which review the literature in depth on thermodynamic properties of limited classes of organic compounds. These also include a critical selection of "best values." These reports are submitted to the Office of Standard Reference Data of the National Bureau of Standards for subsequent distribution to the public.

Status of Work: As of June 30, 1967 the number of valid data sheets extant in the various categories were as follows: physical and thermodynamic properties, 841; infrared spectra, 342; ultraviolet spectra, 126; mass spectra, 192; nuclear magnetic resonance spectra, 611; Raman spectra, 81. On approximately this same date these sheets were being sent to recipients in about 465 organizations scattered throughout the United States and a number of foreign countries.

The above figures represent a 17% increase in valid data sheets and a 32% increase in circulation since the last status report.

Supplements issued during the past year include a revised list of "General References," a new "Introduction" to the Tables of Physical Properties, tables of thermodynamic functions of simple carbon compounds, and a complete survey and selection of critical constants of non-hydrocarbon organic compounds.

The first report to the Office of Standard Reference Data, "Thermodynamic Properties of Pure Aliphatic Alcohols. Part I. General Introduction, Bibliography, and Properties of Eight Normal and Branched Alkanols, C₁ to C₄" has been completed. It is anticipated that Part II, on the remaining aliphatic alcohols, will be completed soon.

Future Plans: Supplements of data sheets on Physical and Thermodynamic Properties will be issued, as in the past. Emphasis will be placed on basic thermodynamic data of aliphatic alcohols, simple carbon compounds, halo-alkanes, and aliphatic ketones.

A study of efficient means of tabulating data of mixtures is now underway and will continue. An increased output of spectral data sheets is anticipated. A complete computer generated index of all compounds contained in all categories of both the API Research Project 44 and the TRC Data Project is in preparation, and should be completed within a few months.

The next NSRDS-NBS report will cover the thermodynamic properties of aliphatic ethers.

3. Title: Molten Salts Data Center

Location: Rensselaer Polytechnic Institute, Troy, New York 12181

Principal Investigator: George J. Janz

Date Initiated: June 1965

Technical Scope: Critical evaluation of data of molten salts, continuing literature searches and information retrieval, continuing upgrading of information now available.

Properties and Species: Inorganic compounds in the molten state; properties: electrical conductance, viscosity, density, surface tension, and emf (formation cells). Extension to additional physical properties is projected.

Products Issued: (a) Molten Salts: Electrical Conductance, Density, and Viscosity Data (172 compounds as single-salt melts), by G. J. Janz, F. W. Dampier, and P. K. Lorenz, Rensselaer Polytechnic Institute, NSRDS-NBS-15, in press, (b) Molten Salt EMF Formation Cells, by Chr. G. M. Dijkhuis, Ria Dijkhuis, and G. J. Janz, Chemical Reviews (accepted for May 1968), and (c) Molten Salts Handbook, (Book) 588p + xii, by G. J. Janz, Academic Press, New York (September 1967). (This publication falls within the area of interest of the present mission at Rensselaer as a molten salt data center, but was not prepared under the NSRDS Contract.)

Status of Work: The critical evaluation of the data for the conductance, density, and viscosity of inorganic compounds as single-salt melts has been continued from the viewpoint of upgrading the data and extension to additional compounds; the results in this area for 172 inorganic compounds have been reported in NSRDS-NBS-15.

The surface tension data of inorganic compounds as single-salt melts is being critically evaluated; a technical report giving the recommendations and results for some 106 compounds has been completed.

A critical evaluation of the EMF (formation cells) data is in progress; the scope of this study has been limited to the emf data of binary molten salt mixtures with a common ion from equilibrium-type electrochemical cells. The results will include critically evaluated free energies and excess free energies, as well as emf data.

Work has been initiated on a system for storage and retrieval of the molten salts literature and data using the computer facilities at Rensselaer so that our resources can be of greater service to the National Bureau of Standards Reference Data System for inter- and intra-communications.

Future Plans: The continuing literature study and information retrieval, assessment of experimental methods, and computer calculations will be continued to grade the data relative to the physical properties within the scope of this mission for molten inorganic compounds. As well as the data for systems as single-salt melts, the problem of recommendations for the physical properties of mixtures (e.g., eutetics) will be considered in the next 12 month period. Additional emphasis will also be given to improvements in the data storage and retrieval procedures, utilizing the Rensselaer computer facilities, so as to make the resources at Rensselaer of greater service. Significant advantages to be gained in this area are that the updating of the bibliographies can be much more efficiently achieved and the retrieval of essential information will be more rapid and at less cost. A further projection in this area would be to computerize the critically evaluated data and the temperature dependent equations for the various physical properties of inorganic compounds in the molten state.

List of reports or other products to be issued:

- (a) Molten Salts: Surface Tension Data, by G. J. Janz and J. Wong (anticipated as an NSRDS-NBS publication).
- (b) Electrochemistry of Molten Salts: Free Energies and Excess Free Energies From Equilibrium-Type emf Cells, by Chr. G. M. Dijkhuis and G. J. Janz (anticipated as an NSRDS-NBS publication).
- (c) A series of five (5) manuscripts reporting on the data assessment and results for the properties of electrical conductance, density, viscosity, surface tension; to be prepared for publication in the professional society journals.
- (d) A technical report and/or manuscript reporting on the information storage and retrieval systems, and the use of the Rensselaer computer facilities for this purpose; to be prepared for publication in a professional society journal.

Comments: For the more detailed data compilations, such as the critically evaluated results prepared under the NSRDS mission, there are no adequate existing journals, so that the NSRDS publication series under the U.S. Department of Commerce is the only outlet for prompt publication and availability. To cope with inquiries received from the technical community at large, some additional approach, suited for rapid and efficient information retrieval per specific inquiries, seems very important. For this purpose we feel the computer-methods presently being considered at Rensselaer promising and important.

There should be some professional journal devoted to complete tabulation of original data and pertinent experimental details; existing journals appear quite inadequate for this purpose, and the mission of

a program such as the NSRDS program would benefit greatly from such publications.

4. Title: Thermodynamic Properties of Ammonia

Location: Heat Division, Equation of State Section, IBS, NBS

Principal Investigator: Lester Haar

Date Initiated: January 1966

Technical Scope: The object of this program is to obtain accurate and consistent tables of thermodynamic properties of ammonia. In this connection, the NBS Circular 142, "Tables of Thermodynamic Properties of Ammonia," first issued in 1923, is to be revised and brought up-to-date. Today ammonia is a far more important material than it was in 1923 when its prime application was in the refrigeration industry (1966 production was about 10 million tons); it is now used in industries unheard of at that time. Also, today's engineer is more sophisticated than the engineer of 1923. He requires more accurate data over broader ranges and at more closely spaced intervals. It is to satisfy this need that this work is directed.

Properties and Species: Thermodynamic functions will be tabulated as a function of temperature and density. These include Gibbs Free Energy, Enthalpy, Heat Capacity, and Entropy. Following the treatment of ammonia, it is hoped to similarly treat other polar gases, such as HF and steam.

Products Issued: "Thermodynamic Properties of Ammonia as an Ideal Gas," by L. Haar, NSRDS-NBS-19, in press. This work represents a significant improvement over that previously available for this complicated species.

Status of Work: The extension of the ideal gas properties to the properties of the real gas is now in progress and an early publication of some of these results is anticipated.

Future Plans and Comments: Following the treatment of ammonia, it is planned to similarly treat the thermodynamic properties of other polar gases, such as HF and steam. As with ammonia, the use of these materials has been increasing at a tremendous rate, and with this the requirements of the modern engineer for accurate thermodynamic properties. These needs are aggravated by the apparent long neglect of this important field. As an illustration, in their recently published book Reid and Sherwood^{1/} lament the lack of study in this area and the general lack of quantitative properties, such as needed by the modern engineer.

^{1/} Robert C. Reid and Thomas K. Sherwood, The Properties of Gases and Liquids, McGraw-Hill Chemical Engineering Series, Second Edition, 1966.

5. Title: Low-Temperature Specific Heats Data Center

Location: Institute for Basic Standards, NBS

Principal Investigator: G. T. Furukawa

Date Initiated: 1963

Description of Project: The center is concerned with the evaluation of best values of specific heats of pure substances from 0 to 300 K with emphasis on the values at the lower temperatures. The information is needed in the correlation of theories and observations of various physical properties. The first objective is the evaluation of the best values of specific heats of the elemental species. This will be followed by the oxides, halides, and others. As an adjuvant effort, the center will maintain as complete as practical a file of specific heat data. The center maintains close cooperation with bibliography centers.

Properties and Species: Partly given above. The high-temperature relative enthalpy data are also examined to determine the best values of specific heat around 300 K. The derived thermodynamic properties (entropy, Gibbs energy, and enthalpy) are calculated also from the results of the critical analysis. The data on the elements: V, Nb, Ta, Fe, Co, Ni, Cr, Mo, W, Os, Ir, and Pt are at present being correlated.

Products Issued: Critical Analysis of the Heat-Capacity Data of the Literature and Evaluation of Thermodynamic Properties of Copper, Silver, and Gold From 0 to 300 °K, by G. T. Furukawa, W. G. Saba, and M. L. Reilly, NSRDS-NBS-18, is in press.

Status of Work: Plots of the specific-heat data on all of the elements and card punching of about 60 percent of the data have been completed. Over 12,000 papers on heat data and related information essential for the analysis are now on file.

Future Plans: (Partly given above under Properties and Species.) The data on Ru, Rh, Pd, Zn, Cd, Hg, Ba, Al, Ga, In, Tl, Ge, Sn, and Pb will be analyzed after those listed in Description of Project are completed. The work on Cr, Mo, W, Os, Ir, and Pt should be completed soon.

Comments: The work of the Center will be helped if authors of papers and reports on specific heats and relative enthalpy would send reprints to the Center. If the actual observations are not published, then they should preferably accompany the reprints sent to the Center.

6. Title: High Pressure Data Center

Location: Brigham Young University, Provo, Utah 84601

Principal Investigator: H. Tracy Hall

Date Initiated: September 1965

Description of Project: The current projects are: (a) An evaluation of experimental data and equations of state relating to the definition of a pressure scale principally in the range up to 100 kbar. This evaluation includes a discussion of fixed points on the pressure scale, interpolation devices and extrapolation formulas. (b) The Data Center keeps up-to-date bibliographic and document files on all papers published in the area of high pressure research. This file is computerized in the KWIC format. (c) Compilation of phase diagrams and crystal data on all materials studied at high pressure and temperatures.

Properties and Species: The present work is chiefly concerned with equilibrium transition pressures of liquid \rightleftharpoons solid and solid \rightleftharpoons solid phase transitions up to 100 kbar. Crystal structure data of high pressure polymorphs is also being compiled.

Products Issued: The report of the current year's study, "An Evaluation of the Pressure Scale up to 100 kbar," will be issued soon. A Directory of High Pressure Workers is being compiled and should also be ready soon.

Status of Work: In the 1966-1967 project year, an evaluation of experimental data and empirical equations of state relative to pressure calibration has been completed. Bibliography and reprint files are being maintained on a current basis. Up-to-date addresses are also kept on high pressure researchers along with information regarding their field of specialization.

As of June 1967, the Center began a compilation of phase diagrams and crystallographic information on all pressure induced structures.

Future Plans: (a) Evaluation of pressure scale at high temperatures which will include a discussion of triple points, phase boundaries, and equations of state applicable at high pressures and temperatures. (b) Evaluation of compressibility data in the range to 100 kbar. (c) Evaluation of phase boundaries as a function of pressure and temperature; (1) melting (solid \rightleftharpoons liquid), (2) solid \rightleftharpoons solid.

7. Title: High Temperature Behavior of Inorganic Salts

Location: NBS

Principal Investigator: K. H. Stern

Date Initiated: October 1963

Description of Project: This project is concerned with the critical evaluation of those properties of inorganic salts which are significant for their behavior (thermal decomposition) at high temperatures. The resulting publications are intended to answer such questions as "Does

compound X exist at Y °C?," "How fast does it decompose?," etc. Answers to such questions are frequently needed by scientists and engineers interested in utilizing salts at high temperatures.

Species: Inorganic salts with monatomic cations and well-defined oxyanions containing one element in addition to oxygen (sulfates, carbonates, nitrates, etc.).

Properties: Decomposition reactions, free energy functions of reactants, products, and reactions from 298 K up to as high as possible, partial pressures of product gases, phase transitions, densities, kinetics of decomposition, and descriptive material.

Products Issued: High Temperature Properties and Decomposition of Inorganic Salts, Part 1. Sulfates, by K. H. Stern and E. L. Weise, NSRDS-NBS-7, October 1966.

Status of Work: A monograph on carbonates is in preparation. Thermo-dynamic calculations are in progress and the literature, largely Russian and Japanese, on thermal decomposition kinetics is being collected.

Future Plans: The monograph on carbonates will be completed. This project has been terminated.

Comments: In addition to preparing the above monograph we would also like to issue a cross-referenced bibliography of molten salts, based on our file of 3000 McBee Keysort cards. This project will have to wait until the associated computer problems are solved.

8. Title: Thermodynamic Properties of Liquid Metals and Liquid Oxides

Location: Department of Metallurgy and Materials Science, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

Principal Investigator: John F. Elliott

Date Initiated: July 1965

Technical Scope: Elements present at relatively low concentrations in liquid metals are of importance in the extraction and refining of metals, in problems of solidification of metals, and in liquid-metal heat exchange systems. Knowledge of the behavior of impurity oxides in the liquid oxide systems that form metallurgical slags is also of importance in the reduction and refining of metals. A current, critical compilation of the information on these properties is of fundamental value to the field of metallurgical engineering, and it is also of value to those conducting theoretical studies on the basic properties of liquid metals.

Properties Covered: Metals — activities, activity coefficients, free energy and enthalpy, interaction coefficients, partial molar heats of solutions. Oxides — activities and activity coefficients.

Products Issued: Some compiled results have been included in "Heats of Solution of Aluminum, Copper, and Silicon," by F. Woolley and J. F. Elliott, Trans. Metallurgical Soc. AIME, in press, and in several recent papers in Trans. Metallurgical Soc. AIME, by J. Chipman and J. F. Elliott, which deal with the properties of alloyed liquid iron. Tabulations of critically evaluated interaction coefficients for iron, nickel, copper, and some lesser metals are in preparation.

Status of Work: Evaluation of data is continuing on a reduced level for the current project year. The current literature is being kept under surveillance. In the past six months considerable attention has been devoted to determining the best mathematical formalism for correlating the data on metallic solutions.

Future Plans: A technical publication covering the problem of the means for correlating the properties of solute elements in liquid metals is in preparation and will be submitted for publication soon. A tabulation of critically appraised interaction coefficients for elements dissolved in liquid iron is planned to be issued this project year.

9. Title: Accumulation and Evaluation of Data on Phase Behavior in Binary and Multicomponent Systems at Elevated Pressures

Location: Chemical Engineering Laboratory, California Institute of Technology, Pasadena, California

Principal Investigator: Bruce H. Sage

Date Initiated: February 1, 1966

Date Terminated: April 30, 1967

Description of Project: The program is concerned with the review and critical evaluation of available experimental data concerning the phase behavior of binary and multicomponent systems at elevated pressures. Such information is of value to practicing engineers in connection with the evaluation of the phase behavior of heterogeneous systems involved in processing operations. An attempt is being made to produce tabular results in sufficient detail that simple four point interpolation will permit the behavior of the system to be evaluated within the accuracy of the primary data. The program has been supported entirely by the Office of Standard Reference Data of the National Bureau of Standards.

Properties and Species: The initial work was directed to a critical review of the phase behavior of the methane-n-pentane system and was followed by a similar review of data pertaining to the phase behavior n-pentane. The information has been extended through the two-phase region

of the above-mentioned binary system at temperatures above 100 °F.

Products Issued: The most advantageous approach to the publication of the extensive tabular information is being developed with the Office of Standard Reference Data. The tabular results for the methane-n-pentane system and for n-pentane have been submitted for comments to the Editorial Review Board and their recommendations are now being incorporated in the above-mentioned manuscript.

Status of Work: The bibliography for n-pentane has been completed and work is now in progress on a much reduced scale upon revising the manuscripts upon methane-n-pentane and upon n-pentane into the form recommended by the Editorial Review Board.

Future Plans: When active work is resumed it will continue upon the accumulation of data and a critical review for the methane-n-butane and the methane-n-decane system. These systems were chosen in order that work could be undertaken upon the methane-n-butane-n-decane system in the near future.

Comments: The program is currently directed to binary and ternary hydrocarbon systems since the principal investigator has had more experience with these compounds and their mixtures than in connection with other binary or ternary systems. The future progress to be expected is primarily dependent upon the availability of support.

10. Title: Critical Evaluation and Selection of the Most Reliable Information on Vapor-Liquid Equilibrium in Binary Mixtures of Non-Electrolytes at Low Pressure

Location: University of Detroit, Department of Chemical Engineering, Detroit, Michigan 48221

Principal Investigators: Leon S. Kowalczyk and Lawrence N. Canjar

Date Initiated: January 15, 1967

Technical Scope: A literature search is being made for all the relevant data pertaining to all binary systems of non-electrolytes measured at low pressures (less than two atmospheres). These data will be compared, critically evaluated and correlated with suitable equations to produce a smoothed, internally consistent, set of thermodynamic and physical properties.

Properties Covered: For each system the following properties will be studied: (1) Vapor pressure of pure compounds, (2) vapor and liquid compositions of co-existing phases, (3) vapor pressures of liquid mixtures, (4) azeotropic states, (5) enthalpy and volume changes of mixing, (6) heat capacities of liquid and vapor mixtures, and (7) miscibility data. All non-electrolytes will be considered.

Products Issued: This project has just begun and therefore no completed reports have been produced.

Status of Work: At the present time vapor pressure data have been studied and techniques for correlation and selection have been tested.

Future Plans: Compositions of co-existing phases are now being collected for the development of techniques for their correlation and critical evaluation. The first system under study is benzene and acetone. This will be followed by systems involving acetaldehyde and other organic compounds.

11. Title: Properties of Electrolyte Solutions Data Center

Location: NBS

Sponsor: NASA

Principal Investigator: Walter J. Hamer

Date Initiated: October 1964

Description of Project: Critical evaluation of published data on electrolytic conductivities, transference numbers, ionic mobilities, activities and activity coefficients of electrolytes in aqueous and non-aqueous media and of the electromotive forces and electrode potentials of galvanic cells made with aqueous and non-aqueous solutions.

Properties and Species: This is not a list of properties. The properties are given in the Description of Project.

Products Issued: Final results are issued in the form of quarterly reports and sent to the sponsor, NASA. Five quarterly reports have been issued to date. Related work and reports being done for NASA are the following:

"Electrochemical Studies in Nonaqueous Solvents. I. Acetonitrile," by L. M. Gedansky and K. S. Pribadi of the Carnegie Institute of Technology.

"Oxidation Potentials for Some Transition Elements," by Loren G. Hepler, Carnegie Institute of Technology.

Status of Work: To date progress has been considerably delayed owing to lack of staff. It is expected that this situation will be improved by the addition of Dr. Yung-Chi Wu to the staff.

Future Plans: The work on subjects included under Properties and Species will be pushed as fast as possible.

12. Title: Thermodynamic Properties of Metals and Alloys

Location: Lawrence Radiation Laboratory, Berkeley, California 94720

Sponsor: U.S. Atomic Energy Commission

Principal Investigator: Ralph Hultgren

Date Initiated: 1955

Technical Scope: Thermodynamic data for all metals, their alloys, and some related semi-metallic systems.

Properties and Species: All standard thermodynamic functions, thermal functions, vapor pressures, B.P., M.P., activities, activity coefficients, partial molar quantities.

Products Issued: Selected Values of Thermodynamic Properties of Metals and Alloys, John Wiley, 1963. This text is under revision. The Center also produces data sheets when appropriate and distributes them free of charge.

Status of Work: This Center is a continuing project funded by the U.S. Atomic Energy Commission.

13. Title: Binary Metal and Metalloid Constitution Data Center

Location: Illinois Institute of Technology Research Institute, Chicago, Illinois

Sponsor: AEC, NASA, USAF

Principal Investigators: F. A. Shunk and N. M. Parikh

Date Initiated: June 1967

Technical Scope: The primary purpose of this center is to search and review the literature and publish critically reviewed binary alloy phase diagrams.

Properties and Species: Constitution diagrams.

Products Issued: Annual reports and possibly hard-bound books.

Status of Work: The abstract search for all binary systems from Ac-Ag to Au-Zr will be completed by the end of October 1967. This will cover all published references for these systems up to mid-1966. The

critical reviews on these systems will be initiated immediately after acquisition of all the papers.

Future Plans: A complete report containing critical reviews of the systems mentioned above will be issued in July 1968. During this period, abstract searches will be initiated for binary systems of B-Ba to Om-O for next year's reviews. Cumulative reference cards for the first year's reviews are projected to be about 4500 and those for the second year to be about 7500.

Comments: This center will supply references on specific systems at its convenience to any bonafide scientist.

14. Title: Thermodynamic Functions of Cryogenic Fluids

Location: Cryogenic Data Center, Cryogenics Division, Institute for Materials Research, NBS, Boulder, Colorado

Sponsor: NASA

Principal Investigators: H. M. Roder, R. D. McCarty, and V. J. Johnson

Date Initiated: Continuing program.

Technical Scope: The project is concerned with compilation, critical evaluation, and dissemination of the thermophysical properties of cryogenic fluids. We attempt the reconciliation of diverse sources of experimental data such as P-V-T, virial coefficients, specific heats, velocity of sound, and Joule-Thomson coefficients. The products are tables and charts which are used by scientists and engineers everywhere in design and applications ranging from refrigeration to space age propellant to legislative standards.

Properties Covered: Statistical specific heats, vapor pressure data, virial coefficients, P-V-T, internal energy, enthalpy, entropy, specific heats at constant volume, constant pressure and their ratio, velocity of sound, and Joule-Thomson coefficients. (Standard state is 0 K.) For additional properties see Comments below.

Species Being Investigated: Active: hydrogen, normal and para, deuterium, argon, helium, methane. Inactive: oxygen, neon, nitrogen, carbon monoxide.

Products Issued: The Thermodynamic Properties of Oxygen, by R. B. Stewart; Ph.D. Thesis, University of Iowa, Iowa City (June 1966). The Thermodynamic Properties of Deuterium, by R. Prydz; M.S. Thesis, University of Colorado, Boulder, Colorado (April 1967).

Status of Work: For hydrogen we are extending the coverage of values tabulated in NBS Monograph 94 to include the temperature range from 100 to 700 K. The thesis on deuterium is being changed to a format

suitable for an NSRDS monograph. Previous work on argon has been extended and reworked also for presentation as an NSRDS monograph which is nearly completed. Thermodynamic charts of argon for inclusion in the monograph have been completed. Analysis of P-V-T and heat capacity data on helium to extend temperature and pressure ranges of previous tabulations is about halfway completed. A bibliography of papers on the properties of methane is close to completion.

Future Plans: Publication of a monograph or IUPAC tables for hydrogen. Publication of a monograph on the thermal functions of oxygen. Publication of a monograph on the thermal functions of helium. Analysis of the P-V-T and specific heat data of methane for preparation of tables and charts over the range from triple point to room temperature. Survey and publication of a bibliography on the available papers pertaining to properties of air.

Comments: The project is responsive to national and international needs as evidenced by (1) designation of the Cryogenic Data Center as the national center for information on properties of materials at cryogenic temperatures, (2) cooperation in the Thermodynamic Tables Project Center of IUPAC, (3) advice to Compressed Gas Association, and (4) support by NASA for its needs and the needs of its contractors.

Compilation efforts are complemented by an extensive experimental program within the Cryogenics Division. Other physical properties studied experimentally or in noncritical collections of data are: dielectric constant, index of refraction, emissivity, surface tension, electrical resistivity, and liquid-solid equilibrium.

The compilation program uses, as a primary tool, the large automated file of documents developed by the Documentation Unit of the Cryogenic Data Center. From this file of documents, papers on specific subjects can easily be retrieved. Input to the tape file provides the basis for our current awareness service, while the file itself plays an important role in our answering service.

Cooperation with other compilation centers or similar activities such as the Helium Research Center, the Los Alamos Scientific Laboratories, and the NBS Heat Division is extensive.

15. Title: Thermophysical Properties Research Center (TPRC)

Location: Purdue University, 2595 Yeager Road, West Lafayette, Indiana 47906

Principal Investigators: Y. S. Touloukian (Director), C. Y. Ho, and R. W. Powell

Date Initiated: TPRC founded January 1, 1957; NSRDS project initiated June 1, 1964

Technical Scope: This Research Center provides comprehensive and authoritative source information on the thermophysical properties of all matter through thorough search and collection of the world literature, generates critical tables of standard reference data through integrated programs of compilation and critical evaluation of existing data, theoretical studies, and experimental determinations, and conducts basic research on thermophysical properties of materials. Only the project on the critical evaluation of existing data, a small part of the overall programs, receives its financial support from the NBS Office of Standard Reference Data.

Properties and Species: World literature search and documentation on 16 properties of all matter at all temperatures. The properties under above scrutiny are: thermal conductivity, accommodation coefficient, thermal contact resistance, thermal diffusivity, specific heat, viscosity, emissivity, reflectivity, absorptivity, transmissivity, solar radiation coefficient, Prandtl number, diffusion coefficient, thermal linear expansion, thermal volumetric expansion, and surface tension. Data compilation and Data Book publication on 10 properties, namely: thermal conductivity, thermal diffusivity, specific heat, viscosity, emissivity, reflectivity, absorptivity, transmissivity, thermal linear expansion, and thermal volumetric expansion. The project on the critical evaluation of existing data and generation of recommended reference data covers currently the thermal conductivity of elements, oxides, liquids, and gases at all temperatures from absolute zero to the highest temperature measured, and specific heat of liquids and gases.

Products Issued:

- (a) Thermal Conductivity of Selected Materials, by R. W. Powell, C. Y. Ho, and P. E. Liley, NSRDS-NBS-8, November 1966.
- (b) Thermal Conductivity of Selected Materials, by C. Y. Ho, R. W. Powell, and P. E. Liley, NSRDS-NBS-16, in press.
- (c) TPRC Data Book, Volume 1, Metallic Elements and Their Alloys — Thermal Conductivity, Radiative Properties (Emissivity, Reflectivity, Absorptivity, Transmissivity), Thermal Diffusivity, and Specific Heat, published since 1960 with supplemental releases (additions or revisions) issued twice yearly, 1578 pages as of December 31, 1966.
- (d) TPRC Data Book, Volume 2, Nonmetallic Elements, Compounds, and Mixtures (in Liquid or Gaseous State at NTP) — Thermal Conductivity, Viscosity, and Specific Heat, published since 1960 with supplemental releases issued twice yearly, 571 pages as of December 31, 1966.
- (e) TPRC Data Book, Volume 3, Nonmetallic Elements, Compounds, and Mixtures (in Solid State at NTP) — Thermal Conductivity, Radiative Properties (Emissivity, Reflectivity, Absorptivity, Transmissivity), Thermal Diffusivity, and Specific

Heat, published since 1962 with supplemental releases issued twice yearly, 1173 pages as of December 31, 1966.

- (f) Touloukian, Y. S. (Editor), Thermophysical Properties of High Temperature Solid Materials, in 6 volumes and 9 books with 15 properties reported, 8479 pages, MacMillan Co., 1967.
- (g) Touloukian, Y. S. (Editor), Thermophysical Properties Research Literature Retrieval Guide, in 3 books with 33,700 references for 12 properties of 45,116 substances, 2700 pages, Plenum Press, 1967.
- (h) Masters Theses in the Pure and Applied Sciences, Volumes 1 to 11, published one volume per year since 1957.
- (i) Inquiry answering and consulting services.

Status of Work: For more than ten years TPRC has been conducting integrated continuing programs of literature search, bibliographic information organization and documentation, data compilation and critical evaluation, and theoretical and experimental research on thermophysical properties. All phases of the programs are fully operational and TPRC has been undergoing expansion every year in all phases of its activities. In the project on the critical evaluation, analysis, and synthesis of existing data supported by the NBS Office of Standard Reference Data, since the completion of the work on the thermal conductivity of 29 selected materials as potential calibration standards, a systematic program has been underway. The work on the thermal conductivity of the elements (experimental data are available for 82 of the 103 elements) is being completed and the work on the thermal conductivity of metal oxides and on the specific heat of 56 fluids (in both liquid and gaseous states) is in progress.

Future Plans: This Research Center's integrated overall programs will be continuously expanded. In the project on the critical evaluation of existing data it is planned in the near future to initiate work on the thermal conductivity of binary and multiple alloys and the specific heat and the radiative properties of the elements (solid state). Initiation of work on the thermal conductivity of binary gas mixtures is also contemplated. A hard-bound volume on the thermal conductivity of elements will be published next year.

Comments: This Center is one of the pioneers among data analysis centers. It is unique in that its total activities are devoted to thermophysical properties research and the advancement of knowledge in this area to better serve education, science, and technology, through completely integrated comprehensive programs. This Center also is the official DoD Information Analysis Center on thermophysical properties. To implement its claim to comprehensive coverage, TPRC operates two overseas Divisions, one in Kobe, Japan, and the other in Brussels, Belgium.

16. Title: Viscosity and Thermal Conductivity of Mixtures in the Gaseous and Liquid States

Location: Northwestern University, Evanston, Illinois

Sponsor: Office of Standard Reference Data, NBS

Principal Investigator: George Thodos

Date Initiated: February 8, 1967

Technical Scope: Viscosity and thermal conductivity measurements available in the literature for gaseous and liquid mixtures are being collected and evaluated to establish dependable values for these transport properties. These selected values will then become accessible for studies aimed to determine methods of correlation for their generalized prediction from pure component values.

Properties and Species: The present investigation has centered in the treatment of gaseous mixtures of nonpolar substances. Future work will be extended to include mixtures of polar substances.

Products Issued: None.

Status of Work: The initial phase of this investigation is considering the development of a method for the prediction of viscosities of gaseous mixtures at normal pressures from information available from their pure components. With regard to this, viscosity information available at normal pressures for pure components has been applied and extended to mixtures. In this connection, a number of binary mixtures, including some with helium and hydrogen, have been treated to establish interaction coefficients which allow prediction of non-ideal behavior of these binary mixtures. The procedure developed reproduces experimental values with an accuracy of about two percent. Presently, this information is being compiled in a Master of Science thesis and a manuscript.

Work to date on this project has concentrated on the procurement of references pertinent to this project. To this end, the Retrieval Guides, Volumes I, II, and III, of the Thermophysical Properties Research Center of Purdue University were extensively utilized to supply information current through 1960. In addition, a computerized literature search covering the transport properties of mixtures of the monatomic and diatomic gases has been obtained from the Cryogenic Data Center of the National Bureau of Standards at Boulder, Colorado.

Currently, an effort is being made to obtain copies of the literature references pertinent to this project. At this time, a substantial number of these literature references have been obtained and a continuing effort is being made to obtain as many of them as is possible.

Future Plans: A preliminary look at this project points out the necessity of a continuing effort not only to obtain basic information,

but also to use this information for the development of correlative methods that will permit the prediction of viscosity and thermal conductivity of mixtures in their gaseous and liquid states from pure component values. This is accentuated from the considerable lack of such transport property information for a number of systems.

17. Title: Transport Properties of Cryogenic Fluids

Location: Cryogenic Data Center, Cryogenics Division, Institute for Materials Research, NBS, Boulder, Colorado

Sponsor: NASA

Principal Investigators: H.J.M. Hanley and H. M. Roder

Date Initiated: June 1965

Technical Scope: This activity is concerned with transport phenomena in fluids. (Viscosity, thermal conductivity and diffusion.) Despite the work done on this topic and its importance to the scientist and engineer, an adequate understanding of the phenomena and proper evaluated data are still lacking. This is especially true for the dense gas and liquid state. Our object is to study and try to understand the theoretical background with the ultimate result of providing authoritative tables.

Properties Covered: Viscosity, thermal conductivity, and diffusion coefficients. Thermal diffusion. P-V-T data to a lesser extent.

Species Being Investigated: Helium, neon, argon, krypton, xenon, oxygen, nitrogen, hydrogen, methane, carbon monoxide.

Products Issued:

Hanley, H.J.M., National Bureau of Standards Technical Note No. 333 (March 1966), The Viscosity and Thermal Conductivity Coefficients of Dilute Argon Between 90 - 2000 °K.

J. Chem. Phys., 44, 4219 (1966), "Comparison of the Lennard-Jones, Exp: 6 and Kihara Potential Functions Using Viscosity Data of Dilute Argon."

J. Chem. Educ. (in press, 1967), "The Thermodynamics of Transport Phenomena in Membrane Systems."

Hanley, H.J.M. and Childs, G. E., National Bureau of Standards Technical Note No. 352 (March 1967), The Viscosity and Thermal Conductivity Coefficients of Dilute Neon, Krypton, and Xenon.

Childs, G. E. and Hanley, H.J.M., National Bureau of Standards Technical Note No. 350 (October 1966), The Viscosity and Thermal Conductivity of Dilute Nitrogen and Oxygen.

Cryogenics (Submitted), "Applicability of Dilute Gas Transport Property Tables to Real Gases."

Status of Work: Methane, hydrogen, and helium are being investigated with the object of producing tables similar to those produced for the gases mentioned in Products Issued above.

The theoretical investigation is concerned with (a) a clear understanding of the relationships of a theoretical expression and the intermolecular potential function. Three papers are ready for publication on this topic, (b) the transport virial coefficients, (c) modification of theories to assist in correlations of dense gas transport data, (d) possible serious errors in high temperature viscosities.

Future Plans: Publication of tables for hydrogen and methane. Publication of a monograph on the transport properties of the noble gases. Publication of results from section (b), (c), and (d) of Status of Work.

Comments: Please refer to the comments under the project "Thermodynamic Properties of Cryogenic Fluids," carried out at this Center.

18. Title: Thermal Conductivity of Solid Materials at Low Temperature

Location: Cryogenic Data Center, Cryogenics Division, Institute for Materials Research, NBS, Boulder, Colorado

Sponsor: NASA, NBS

Principal Investigators: G. E. Childs and R. L. Powell

Date Initiated: November 1966

Technical Scope: The objective of this project is a complete updating and reissue of NBS Circular 556 by R. L. Powell and W. A. Blanpied. The circular has been out of print since 1961, it covered the literature to 1954, and has been one of our most useful and practical publications.

Properties Covered: Thermal conductivity at temperatures below 300 °K.

Species: Metals, alloys, nonmetallic solids.

Products Issued: None.

Status of Work: An initial survey of the literature has been completed and all applicable documents ordered. Many papers have been received and data from these are being extracted.

Future Plans: Publication of a monograph — essentially an updated version of NBS Circular 556.

Comments: The compilation program benefits from active cooperation with the experimental group in our division which is conducting measurements of thermal conductivity at cryogenic temperatures.

19. Title: Center on Diffusion in Gases and Liquids

Location: Department of Chemical Engineering and Institute of Molecular Physics, University of Maryland, College Park, Maryland 20740

Principal Investigator: J. M. Marchello

Date Initiated: November 1965

Technical Scope: This activity is concerned with the compilation and critical evaluation of diffusivity and viscosity data on gas, liquid, solid and turbulent flow systems.

Properties and Species: Transport properties, especially diffusivity and viscosity.

Products Issued: None.

Status of Work: Staff members are completing and updating their bibliographies and finishing the data evaluations.

Future Plans: Several reports will be issued in the next few months. These include the diffusivity in gases, polymers, and liquids.

VIII. CHEMICAL KINETICS

Compilation, evaluation, and tabulation of numerical data in the field of chemical kinetics presents a number of special problems. By definition, the system is changing in composition; the reaction mechanism may be uncertain, or may change with temperature or other parameters; catalysts, wall-effects and other local influences may be significant. Previous attempts to present kinetic data in tabular form (e.g., NBS Circular 510, Tables of Chemical Kinetics — Homogeneous Reactions, with two supplements, prepared under the direction of N. Thon and Charles Stauffer) have found the difficulties substantial.

To obtain advice on a program which might avoid some of these problems, the Office of Standard Reference Data sought the counsel of the NAS-NRC Committee on the Kinetics of Chemical Reactions. The recommendations of the Committee recognized the difficulties inherent in any undertaking to evaluate and compile in tabular form the large amount of numerical data to be found in the literature on rates of chemical reaction. Instead, the Committee suggested a program of critical review monographs on narrow topics, to be written by qualified specialists. The purpose of these reviews would be to provide comprehensive coverage within the area chosen, with emphasis on the quantitative aspects, and with extensive bibliography.

A number of critical reviews have been started and some are completed: one has been published and several others are in press. The list of projects, which appears below, gives details of the reviews. Experience to date indicates that the critical review approach is valuable, but that the author must be careful to limit the scope of his topic in order to avoid being overwhelmed by the quantity of literature which he must read and analyze.

In addition, it has become clear that both review authors and the user public can be helped greatly by the establishment of information and data centers which function to:

- (a) Provide authors of monographs with bibliographic services and assistance.
- (b) Maintain coverage of the scientific literature on a current basis.
- (c) Store and classify the data and bibliographic content of critical review monographs.
- (d) Provide information to the scientific public on the basis of items (b) and (c).

Two data centers have been established: the NBS Chemical Kinetics Information Center acting in a general capacity, and the University of Notre

Dame Radiation Chemistry Data Center. These centers are at present performing the first two services listed above, and are providing some limited information services to the public as well. Establishment of additional centers and arrangements for additional critical review monographs have been hampered by the limited funds available. The support of the DoD Advanced Research Projects Agency has provided means for partial support of the NBS Chemical Kinetics Information Center. The Atomic Energy Commission has shared in supporting the Radiation Chemistry Data Center.

Descriptions of centers and critical review projects follow.

1. Title: Chemical Kinetics Information Center

Location: Physical Chemistry Division, NBS

Principal Investigator: David Garvin

Date Initiated: December 1962

Description of Project: A center for the collection and dissemination of information on rates of thermal chemical reactions, cross sections of reactive collision processes and quantum yields of photochemical processes. The center locates reports on these processes, indexes them, establishes and maintains a reference file of the reports and a subject index to them, and prepares bibliographies on specific topics.

Properties and Species: Rates, activation energies and preexponential factors for thermal reactions that are homogeneous in the gas, liquid or solid phases. Heterogeneous catalysis and radiochemistry are excluded.

Cross sections of reactive collision and energy transfer processes. Atom-molecule and molecule-molecule processes are covered. Electron-molecule collisions are excluded. (As used here, cross section refers to the probability of a process, determined as a function of energy or for molecules in specific energy states.)

Products Issued: The Center has not issued any works in published form. It prepares and distributes bibliographies on demand. These are prepared for authors of reviews in the NSRDS series of monographs on chemical kinetics and in response to requests from the public. A description of the Center has been published. "Two National Bureau of Standards Data Centers: Chemical Kinetics and Mass Spectrometry," David Garvin and Henry M. Rosenstock, J. Chem. Documentation, 7, 31 (1967).

Status of Work: (a) Bibliographies issued. Twenty-four were distributed in the period from April 1966 through October 13, 1967. (b) Selection and indexing of documents. The Center's index now contains 11,454 documents plus the approximately 5000 items in the IDA Bibliography. Approximately 3600 papers and reports were added to the Center's index in the period April 1966 to October 12, 1967. This work has been

done by the staff of the Center and by other members of the Elementary Processes Section, IBS. (c) An indexed collection of references to reactions of light molecules, prepared under the direction of Dr. Adolf Hochstim, Institute for Defense Analyses, has been transferred to the Center and adapted to its use. This collection is on magnetic tape, and is searched by means of locally developed computer programs. (d) The period March 1967 - October 1967 has been devoted, in large part, to preparations for extensive use of ADP equipment in the processing of input of material to the Center's index, to the retrieval of such information, and in the preparation of bibliographies.

Future Plans: (a) The Center expects to convert its methods for the input of current information from the use of a manual optical overlay system to a magnetic tape stored index. A trial run on about 450 documents has been made. Use of these techniques on a production basis should start shortly. (b) The Center intends to expand its ability to cover the field of chemical kinetics by the use of part-time indexers in the local academic community. Between 3500 and 4000 articles per year must now be scanned and perhaps 2/3 of them indexed. This task is beyond the capabilities of the present staff, and must be sublet. (c) The Center intends to undertake the codification of existing data compilations on the rates of reactions of light molecules, principally those of interest for air pollution, upper atmosphere and rocketry studies, and to expand this codification to include evaluation. This will be done in cooperation with the JANAF subcommittee on tables of chemical kinetics.

Comments: The principal need of the field of chemical kinetics is for up-to-date, continuing evaluation of data. The NSRDS series of monographs, with its emphasis on data, is needed, and should place a high priority on early publication of the current set of monographs and upon expansion to other topics in the field.

The Center, to remain viable, needs an expanded input base, obtainable through the use of more indexers, and the purchase of indexed material from sources such as Chemical Abstracts and the Institute for Scientific Information. Support is also needed, in the way of funds, for the development and maintenance of a computer-based index system.

2. Title: Radiation Chemistry Data Center

Location: Radiation Laboratory, University of Notre Dame, Notre Dame, Indiana 46556

Principal Investigators: Milton Burton, Director, and Alberta Ross, Supervisor

Date Initiated: July 1965

Technical Scope: This activity is concerned with the elementary processes that occur in chemical systems exposed to ionizing radiation

under a variety of conditions. The numerical data from such investigations are either yields of products, measurements of rates of over-all or individual processes, or changes in properties of the system due to irradiation. The specific objectives are (1) the compilation of numerical data on all the chemical systems which have been investigated, and (2) a critical review of data which are available and employed in support of proposed mechanisms. The project especially aims to serve the needs of radiation chemists, but is also of interest to other chemical kineticists, especially to those studying fast reactions.

Properties and Species: Information relating to rates of reactions including specific rates, equilibrium constants, decay time, entropy of activation, cross-section, or probability; activation energy and other Arrhenius parameters; G (yield in molecules/100eV) or M/N (molecules/ion pair); properties of transients including absorption and emission bands, extinction coefficients, and half-lives; parameters describing interactions of radiation and matter including W and LET. Species being investigated are limited to chemically-defined systems (except metals), including solid, liquid, gas and heterogeneous systems made up of organic and inorganic compounds, in the pure state or as mixtures containing two or more components.

Products Issued: A "Weekly List" of papers on radiation chemistry is distributed to a mailing list. Bibliographies and preliminary compilations have been prepared for individuals on such topics as: Radiolysis of olefins, Specific rates of reactions of HO₂, Radiation chemistry of amides and peptides.

Status of Work: A thesaurus for radiation chemistry has been developed and a glossary of terms is in preparation. Recent papers (1966+) are key-worded according to the thesaurus; numerical data (especially G values and kinetic data) are recorded and filed. Searches are being conducted on request. Literature prior to 1966 is covered by an index contributed to the Center by the Dow Chemical Company. Requests for data are answered from the data file, which is complete for all systems since 1966 and for literature prior to 1966, only for water, methanol and aqueous solutions. References, keywords, and secondary references (citations) are being recorded on punched paper tape for eventual computer manipulation.

Future Plans: "A Thesaurus and Glossary of Radiation Chemistry," and bibliographies on (1) the radiation chemistry of methanol, (2) the radiation chemistry of water and aqueous solutions, are in preparation and will be submitted for publication. System design and programming for searching the reference files by computer will be continued; preparation of the "Weekly List" from computer input, and its wide distribution, is planned. Addition of numerical data to the tape record is being studied. Suitable topics and authors for critical reviews will be selected.

Comments: Current demands on the Center indicate the value of providing bibliographies or specific information from the literature to

those who request it. Present emphasis is on establishment of a useful index and data file from the radiation chemistry literature so that information can be quickly provided on demand. Because of the highly empirical and fragmentary nature of the data, a scientist often prefers to evaluate the previous work for himself. Critical reviews of data can be useful if they are prepared by generally recognized experts. The Center has supported the efforts of reviewers who have contributed chapters on various topics to monograph series by providing the reviewers with bibliographies; the Center will continue to provide such assistance.

3. Title: Tables of Bimolecular Gas Reactions

Location: University College of Wales, Edward Davies Chemical Laboratory, Aberystwyth, U.K.

Principal Investigator: A. F. Trotman-Dickenson

Date Initiated: June 1965

Technical Scope: The project has involved the critical tabulation of all bimolecular gas reactions covered by the listing under Properties and Species.

Properties and Species: The survey has covered all bimolecular gas reactions with the exceptions listed below. Only those reactions for which two or more molecules of product are formed were considered. Those in which one molecule of product is formed can be regarded as a reverse of unimolecular reactions and are best dealt with under a survey of this topic. The survey has excluded reactions of oxygen and nitrogen atoms as they are to be the subject of a separate survey. Atoms and molecules in electronically excited states are also excluded. The tables list all rate data in the simple Arrhenius form, the experimental temperature ranges, an indication of the experimental method used and critical comments on the accuracy of the determinations, where the appropriate best values are recommended.

Products Issued: The initial product of this project has been published as NSRDS-NBS-9, Tables of Bimolecular Gas Reactions. This volume covers the literature for the period to December 31, 1965.

Status of Work: Work is continuing to keep the survey up-to-date.

Future Plans: This project hopes to publish a supplement to the first set of tables that will cover the literature to some point during 1968. The exact date will be decided when the size of the supplementary tables can be estimated more accurately.

Comments: It is of great importance that these tables should be maintained up-to-date, as it will be a very considerable task to catch up if any big gap develops. During 1968 the project will be taken over by the United Kingdom Office of Scientific and Technical Information. Method of publication of future reports remains to be decided.

4. Title: Hydrogenation of Ethylene on Metallic Catalysts

Location: Research Institute for Catalysis, Hokkaido University, Sapporo, Japan

Principal Investigator: Juro Horiuti

Date Initiated: Survey was initiated at March 1, 1966 and the full work at August 1, 1966

Technical Scope: This monograph deals mainly with the hydrogenation of ethylene on unsupported metallic catalysts, especially of evaporated films of pure metals. Experimental data on the decline of catalytic activity are first reviewed, describing relevant methods of the experimental investigation. Summaries are then given of the observed kinetics of the hydrogenation and of the different phases of profiles of the reaction. Attempts to formulate a mechanism of the phenomena in question are reviewed, and finally the experimental results of the hydrogenation and its associated reactions, e.g., parahydrogen conversion, H₂-D₂ equilibration and formation of different deuterioethylenes and deuterioethanes, are accounted for systematically on the basis of the associative mechanism proposed by the principal investigator, et al.

Properties and Species:

- (1) Reproducibility of observations.
- (2) Catalytic activity of various pure metals and alloys.
- (3) Reaction kinetics of hydrogenation and its associated reactions.
- (4) Isotopic effect on hydrogenation rate.
- (5) Experimental results of supported and carbided metal catalysts.
- (6) Reaction mechanisms hitherto proposed.
- (7) Statistical mechanical formulation of the associative mechanism and its application.

Products Issued: No product has been issued to date.

Status of Work: The monograph has been completed and accepted by the Office of Standard Reference Data. It will be published as NSRDS-NBS-13. Publication is expected early in 1968.

Comments: The principal investigator has indicated that following the completion of the present monograph, he will use his experience gained in this monograph to determine the desirability of extending the coverage to include catalyzed hydrogenation of olefines other than ethylene.

5. Title: Rate Constants for Gas-Phase Reactions of Neutral Oxygen Species

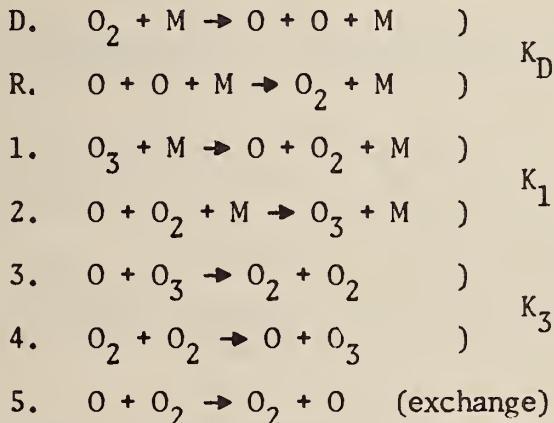
Location: Department of Chemistry, University of California, Berkeley, California

Principal Investigator: Harold S. Johnston

Date Initiated: 1966

Description of Project: The total project was to cover all gas-phase reactions of neutral oxygen species, nitrogen species, and the oxides of nitrogen. To guarantee the completion of a monograph on the project for this calendar year, the scope was reduced to cover all gas phase reactions between three species: atomic oxygen atoms, O ; oxygen molecules, O_2 ; and ozone O_3 . The observed rates of these species are expressed in terms of empirical rate constants and interpreted in terms of a set of seven elementary chemical rate constants. Tables and graphs are given for quantitative studies of these rates, and condensed equations given to represent the data. Certain unusual trends in the data are interpreted in terms of simple gas-phase reaction rate theory.

Properties and Species: The properties covered are: the rate constants for the following elementary reactions:



Insofar as quantitative data are available, tables are given of observed rate constants: k_D , k_R , k_1 , k_2 , k_3 , and k_5 . The relative effect of various inert gases M are given both for the system O_2 and the system O_3 . The thermodynamic equilibrium constants K_D , K_1 , and K_3 are given. The relation of equilibrium constant to rate constants of forward and reverse reaction, where non-equilibrium distributions are known to occur, is examined in detail.

Status of Work: The final report on the oxygen system has been submitted for publication in the NSRDS-NBS series.

Future Plans: With the submission of the report on oxygen species, this work will be terminated.

Comments: This project has been a part of the joint ARPA-NSRDS program for preparation of selected critical reviews.

6. Title: A Critical Review of the Rate Constants of Reactions in Re-entry Flow Fields

Location: General Electric Co., Valley Forge, Pennsylvania

Principal Investigator: M. H. Bortner

Date Initiated: April 1967

Description of Project: For the reactions selected as most important to re-entry flow field kinetics, all available data are being critically reviewed. About fifteen to twenty reactions have been selected on the basis of their importance as judged by past experiences with flow field calculations and current considerations and discussions. The reactions are mainly those of the nitrogen-oxygen system. All data are being carefully considered and, based on these data and the uncertainty therein, a rate constant is being selected for each of the reactions under study. The rate constant is given in the form $k = a T^b e^{-C/T}$ with an uncertainty expressed for each.

Properties and Species: Reaction rate constants for reactions in the nitrogen-oxygen system and some for reactions involving minor species, e.g., Na, H₂O, and CO₂.

Products Issued: A report is to be issued which discusses available data and presents the suggested rate constants and their uncertainties. These data are also to be presented graphically.

Status of Work: Work essentially complete. A rough draft of the report has been prepared. The results are to be discussed and a final report issued.

Future Plans: The review should be continued in two ways. First, it should be continuously updated. Second, the scope of the reactions considered should be increased with information from other critical reviews carried out under NSRDS sponsorship being included in this application of data.

Comments: This project has been a part of the joint ARPA-NSRDS program for preparation of selected critical reviews.

7. Title: Preparation of a Critical Monograph on Quantitative Kinetic Data in the Field of Unimolecular Reactions

Location: Stanford Research Institute, Menlo Park, California 94025

Principal Investigator: Sidney W. Benson, Chairman, Department of Thermochemistry and Chemical Kinetics

Date Initiated: June 1, 1965

Description of Project: Critical summary and review of all quantitative kinetic data on gas phase unimolecular reactions up to about October

1966. Includes criteria for evaluation, estimates of error and independent assignments of "best" rate constants.

Properties and Species: Specific reaction rate constants for elementary decomposition of molecules and radicals.

Products Issued:

- (1) "A Method for Estimating the Arrhenius A-factors for Four- and Six-Center Unimolecular Reactions," by S. W. Benson and H. E. O'Neal, J. Phys. Chem., 71, 2903 (1967).
- (2) "Estimation of Kinetic Parameters for the Pyrolysis of Small Ring Compounds," by S. W. Benson and H. E. O'Neal, in press.
- (3) "Entropies of Polycyclic Rings," by S. W. Benson and H. E. O'Neal, in preparation.

Status of Work: Manuscript in final stages of typing and correction (600 pages).

Future Plans: The manuscript will be completed and submitted for publication with all possible speed.

8. Title: Bibliography of Heavy-Atom Kinetic Isotope Effects

Location: Belfer Graduate School of Science, Yeshiva University, New York, N.Y., and Brookhaven National Laboratory, Upton, L.I., N.Y.

Principal Investigators: Marvin J. Stern, Yeshiva University, and Max Wolfsberg, Brookhaven National Laboratory

Date Initiated: March 22, 1965 [initiated under Contract CST-1288. Contract terminated December 4, 1965. Work continuing without contract].

Description of Project: The bibliography will contain a complete listing of all published papers dealing with theoretical and experimental studies of heavy-atom kinetic isotope effects in in vitro chemical reactions. "Heavy-atom" refers here to all elements other than hydrogen. [A list of "fringe" subjects specifically excluded, and our recommendations regarding these subjects, was given in our last progress report (October 5, 1965).] The bibliography will also contain complete author and cross-referenced subject indices.

Status of Work and Future Plans: Approximately 650 relevant articles, covering the period 1900-1964, have been collected and cataloged. Of these articles, approximately 500 have been indexed. We are in the process of completing the indexing and index-checking of these articles. After com-

pleting this indexing, the literature for the period 1965-1967 will be searched and the additional articles will be included in the compilation. For a number of reasons, work on this project was at a virtual standstill for the last six months. However, production has now picked up again and we anticipate completion in less than one year.

Comments: While it was our original intention to prepare a critical review monograph on this subject, we have decided to stop at the bibliography stage for two pertinent reasons. First, while the number of relevant articles is only about twice that which we originally anticipated, the amount of time necessary for searching the literature is about four times that which we originally anticipated. Our endeavors to date have taken about 8 "man-months" of work; we originally estimated that a complete monograph would take only 9-10 "man-months." Second, and more important, is our strong feeling, after reading several hundred articles containing an abundance of often-contradictory data, that it would not be worth the tremendous amount of time that would be necessary to extract the relevant data from the articles and sensibly tabulate them, let alone critically evaluate them. This statement is not meant to imply that it would be impossible for someone to prepare such a monograph, but that we do not feel that the end result would justify the effort.

9. Title: Bond Dissociation Energies in Simple Molecules

Location: The Catholic University of American, Washington, D.C.

Principal Investigator: B. deB. Darwent

Date Initiated: September 1966

Description of Project: To collect, in tabular form, values of bond dissociation energies published between 1956 and 1966 inclusive. The period 1962-1966 is to be covered more extensively than that of 1956-1962. The material will be restricted to simple inorganic compounds and organic compounds containing not more than one carbon atom, except that the groups $> C=O$ and $- C=N$ are not regarded as being "organic."

All values obtained are being included, regardless of accuracy, and, where feasible, the preferred value is to be given, together with the probable error.

Properties and Species: Bond dissociation energies at 0 K and
298 K.

Status of Work: Manuscript in press.

Comments: The material should be placed on cards, tape or in some system that permits future additions and corrections without the need for retyping.

The rate at which new data are being produced indicates that the

compilation should be brought up-to-date every two or three years.

* * * * *

The following projects, described in the previous Status Report, are no longer active:

- (1) Solvent Effects in Solution Kinetics. Dr. G. C. Akerlof had not completed this review at the time of his death. The material he had compiled and evaluated has been incorporated in the files of the NBS Chemical Kinetics Information Center, and the references are available on inquiry.
- (2) Bibliography of Small Molecules Gas Phase Reactions. The manuscript bibliography is in the hands of the publishers. A computer tape of the references is incorporated in the files of the NBS Chemical Kinetics Information Center.
- (3) Elementary Reactions of the Hydroxyl Radical. Funds to support this review were not available in 1966 or 1967. It remains as a high-priority candidate for reactivation and support by the Office of Standard Reference Data.

In the area of colloid and surface properties, the activities of the Office of Standard Reference Data interact strongly with those of the Committee on Colloid and Surface Chemistry of the National Academy of Sciences - National Research Council. Among other activities the NAS-NRC Committee had started a program aimed at the development of data compilation activities before the initiation of the National Standard Reference Data System and the establishment of the Office of Standard Reference Data. When the Office was established, it began activities in the area of colloid and surface properties by supporting some of the ongoing programs of the NAS-NRC committee. In other cases the NAS-NRC programs did not require support and in still others available resources did not permit support. In any case, the program of the Office of Standard Reference Data bears the strong imprint of the NAS-NRC committee. All but one of the projects in this area were either ongoing or planned NAS-NRC programs. The project which was not, that on the kinetics of phase transformations, reflects a desire to extend the initial program to include some aspects of the physics of surfaces, an area of rapid development in recent years. The subject does, in fact, cover one of the categories of interest of the committee, although one in which there was no active program.

At the present time, the NAS-NRC committee, under the chairmanship of Dr. A. C. Zettlemoyer of Lehigh University, serves the Office of Standard Reference Data in an advisory capacity. The program manager for colloid and surface properties attends the biannual meeting of the subcommittee to report on progress, and to discuss new developments and problems.

Two additions have been made to the program since the previous status report: a project on the critical evaluation of surface tensions of substances which are liquid in the vicinity of room temperature and one on the critical review of data of importance in the interpretation of the kinetics of phase transformation. Details of each are discussed hereafter. The project on surface tensions is an outgrowth of the activities of the NAS-NRC subcommittee; the other involves an extension into surface physics as has been mentioned.

The work on two of the projects has proceeded to the point where the accumulated data or techniques have been cited in technical papers. These are:

"Light Scattering," J. P. Kratochvil, Analytical Chemistry, Annual Reviews, Vol. 38, April 1966, p507R-526R.

"The Meaning and Significance of the Critical Micelle Concentrations of Association Colloids," P. Mukerjee and K. J. Mysels, presented at the 154th National Meeting of the American Chemical Society, Chicago, Ill., September 10-15, 1967.

A final report, Molten Salts: Surface Tension Data, by G. J. Janz and J. Wong, has been received recently and is undergoing review prior to publication. This contains data on 106 inorganic compounds as single-salt melts.

Final reports on the scattering of light by pure liquids and the critical micelle concentrations of association colloids in aqueous solutions are expected in the near future.

Another report containing evaluated data on double layers in systems other than mercury, metals and semiconductors, electro-kinetics and points of zero charge has also been received and is being reviewed. It is planned that the data from this report will be combined with those from other reports yet to come to form a monograph.

Detailed discussions of each project in this area follow.

1. Title: Data Group in the Field of Critical Micelle Concentrations

Location: School of Pharmacy, University of Wisconsin, Madison, Wisconsin 53706, and R. J. Reynolds Tobacco Company, Research Division, Winston-Salem, North Carolina 27102

Principal Investigators: Karol J. Mysels, R. J. Reynolds Tobacco Co., and Pasupati Mukerjee, University of Wisconsin

Technical Scope: Collection of Critical Micelle Concentration (c.m.c.) data, intercomparison and evaluation of experimental methods used, evaluation of c.m.c. data and assignment to various categories of reliability and usefulness, computerized presentation of characterizing pieces of information for easy storage, retrieval, and future expansion.

Properties and Species: The c.m.c. data are for amphipathic, surface-active, compounds in aqueous solution. Variables identified, where possible, are temperature, nature and concentration of additives, and experimental method used (specified in some detail). The species investigated are all manners of amphipathic molecules. These molecules are characterized by the presence of a hydrophobic tail and a hydrophilic head group. The tail is usually an aliphatic chain, which may be branched, may contain aromatic residues, and may be partially or completely fluorinated. The hydrophilic head groups in ionic surfactants are charged and are associated with various counterions. They may also be uncharged, in the non-ionics, or zwitterionic in character. The present list of compounds for which c.m.c. values have already been recorded is 450 in number.

Status of Work: At the time the project was renewed at Wisconsin in November, 1966, some 500 papers had been obtained from a search of the literature. About 2000 c.m.c. values for 305 compounds had been

recorded and evaluated. Since November 1966, about 150 new papers have been obtained and about 150 new compounds and 1600 new c.m.c. values recorded. It is estimated that 90+% of publications to be processed are on hand, and about 75% of the c.m.c. values recorded. An additional 15% or so have been studied in a preliminary fashion before being evaluated and recorded.

Future Plans: Within the next few months it is hoped to bring the project to a conclusion with a cut-off date for the survey of the literature at the end of 1966. The results have been put on computer cards in a form which, with some small changes, should be easy to reproduce in print. It is expected that the results will require a 350-400 page book.

Comments: The c.m.c. values give a quantitative measure of the surface activity of substances in solution, an estimate of the maximum "available" activity of surfactants in solution, and the concentrations where "micelles" appear, with their important role in fundamental studies as "model" colloids and "model" interfaces, and the practical role in the industry as solubilisers and media for reactions. C.m.c. values are of interest to many university scientists working, for example, in departments of chemistry, biochemistry, medical sciences, pharmacy, agriculture, dairy sciences and mineral engineering. In the industry, quite aside from the detergent and pharmaceutical industries, c.m.c. values are useful wherever surfactants are used for foams, froth, emulsions, suspensions, and surface coatings.

There is, thus, a very widespread interest in c.m.c. values. The NSRDS project is attempting not only a critical survey of the "best" data, but also a fairly exhaustive survey of all directly available numerical data and data that can be obtained from personal communications from authors, and retrieved from the literature, either from graphs and equations, or from high quality solution data which yield c.m.c. values after plotting and analysis. Thus, many of the c.m.c. values obtained are "new" in the sense that the numerical values were not directly available.

It is desirable, for these reasons, that the publication of the NSRDS survey should be in a form which will enable scientists and technologists of a wide range of interests to be quickly aware of it and easily avail of it.

The literature in the field continues to grow at a rapid rate. In particular, many interesting new compounds are being synthesized and studied. It is also expected that some sources for the period covered will have been missed and will be unearthed later. After the present project is brought to an end, additional surveys are desirable at intervals of 2-4 years.

2. Title: Electric Properties of Interfaces

Location: Coordination Center: Laboratory for Physical and Colloid Chemistry, Agricultural University, De Dreijen 6, Wageningen, Netherlands

Principal Investigator: J. Lyklema

Date Initiated: April 1, 1965

Technical Scope: The collection and critical evaluation of properties mentioned directly below.

Properties and Species: Properties: Capacitance of charge of the electrical double layer, electrocapillary curves, electrokinetics, including surface conductance points of zero charge. Species: All species that are well defined, that can be reproducibly obtained and on which one of the properties mentioned above is measured in a way meeting our criteria.

Products Issued: Progress reports: (1) December 1965, containing an uncritical compilation of references, (2) October 1966, containing a first selection of references, and (3) November 1967, containing a first selection of critically evaluated data.

Status of Work: Continuation of the critical evaluation of the references mentioned above.

Future Plans: The production of three progress reports, each covering a collection of data in such a way that after completion of the last (sixth) report the whole field will be covered.

Comments: At this moment we are in a period of sustained effort, implying that we have no wish or need except for the possibility to continue the project till completion.

3. Title: Molten Salts Data Center

Location: Rensselaer Polytechnic Institute, Troy, New York 12181

Principal Investigator: George J. Janz

Date Initiated: June 1965

Description of Project and Properties Covered: Evaluation of data on the surface tension of melts of inorganic salts. This project is one task of the Center. A complete description of the Center and all of its tasks is given in the section on Thermodynamic and Transport Properties.

Products Issued: Molten Salts: Surface Tension Data, by G. J. Janz and J. Wong, a report containing data on the surface tensions of 106 inorganic compounds as single salt melts, in press.

4. Title: Light Scattering Critical Data Center

Location: Clarkson College of Technology, Potsdam, New York 13676

Principal Investigator: Josip P. Kratochvil

Date Initiated: April 1, 1965

Description of Project: The Center is established for the purpose of collecting and evaluating data produced in the area of light scattering.

Properties and Species: Properties: Rayleigh ratios and depolarization values; refractive index increments; wavelength and temperature dependence of these quantities; calibration and correction factors in measurements of these quantities; related theoretical aspects. Species: Gases, liquids, liquid mixtures, solutions, and dispersions; electrolytes, polymers, detergents, colloids.

Products Issued: A state-of-the-art review published in Analytical Reviews, by J. P. Kratochvil, "Light Scattering," Analytical Chemistry, Vol. 38, p517R-526R (1966).

Status of Work: Collection and critical evaluation of Rayleigh ratio and depolarization values for liquids and liquid mixtures has been completed. A manuscript for submission to NBS for publication is being readied.

The collection and classification of the refractive index increments of polymers and other solutes is largely completed. The data are being evaluated.

Another state-of-the-art review on light scattering, covering 1966 and 1967, is in preparation for Analytical Reviews.

Future Plans: Manuscripts of two monographs — one on scattering by liquids and liquid mixtures, the other on refractive index increments of polymers and other solutes, will be submitted to NBS for publication.

A review on light scattering covering 1966 and 1967 will be submitted to Analytical Reviews.

The work will continue along lines outlined in the original proposal, with emphasis on scattering by gases.

Comments: Reprints of the review listed under Products Issued above are available from the author.

5. Title: Literature Survey, Evaluation, and Compilation of Surface Tension Data of Pure Liquids

Location: Wayne State University, Detroit, Michigan

Principal Investigator: Joseph J. Jasper, Professor Emeritus

Date Initiated: January 1, 1967

Description of Project and Status of Work:

Initial Procedure: The Decennial Indexes of the Chemical Abstracts were reviewed and all references to the surface tension of liquids tabulated. This was followed by a careful reading of each abstracted title to determine as far as possible if the material therein was pertinent to the data survey.

Data Evaluation: The evaluation of surface tension data involves first of all a careful reading of the journal article describing experimentation and results. The Writer has frequently found it helpful to communicate with the principal author for clarification or for additional information. The quality of surface tension data of a given liquid compound is largely dependent upon (a) the method used (by choice or necessity), (b) degree of purity of the liquid compound, (c) experimentation, i.e., construction of apparatus, temperature control, etc., (d) the scientific reputation and experience of the operator, and (e) the precision measure. The latter is important, and most authors include this value in their reports. However, a large precision measure cannot always be used as the final criterion for the rejection of a series of surface tension data versus temperature data.

Data Processing and Compilation: The Writer has reviewed some 125 journal articles to date and processed the surface tension data from 103 of them. By "processing" is meant that all data were corrected by applying the method of least squares to obtain the most probable values over the given temperature range. This is, of necessity, a slow and tedious process and the average time required for a set of data at 8 to 10 temperatures is about 60 minutes with the aid of a desk computer. The resulting least-squares equation is applied to the original data to determine the magnitude and direction of the deviation of each surface tension value from the most probable one at the given temperature. The equation is now applied for the calculation of a series of surface tension values at whole-number temperatures over the range given in the journal article. The surface tension values are then tabulated as a function of the temperature. The resulting table gives (a) the surface tension at the various temperatures, (b) the method used for measuring the surface tension, (c) the precision measure, and (d) the least-squares constants. To date, 990 compounds have been processed as described above. The results are presented in a series of tables.

Future Plans: The data processing and compilation, as described above, is a continuing operation and will be applied to all liquid compounds selected. Most of the surface tension data so far processed are the only ones available in the literature. Whenever surface tension measurements of a given compound are reported by more than one

author, the Writer will continue to judge the quality of each set of data, as described under Data Evaluation. Many more liquid compounds remain to be considered.

6. Title: Evaluation of Physical Data Pertaining to Phase Transition Kinetics

Location: Materials Science Department, Stanford University, Stanford, California

Principal Investigators: G. M. Pound and W. A. Tiller

Date Initiated: May 1, 1967

Technical Scope: A critical review and evaluation of the physical data pertinent to phase transition kinetics, i.e., to nucleation and growth in condensation, evaporation, freezing, etc.

Properties Covered: Coefficients of evaporation of liquids and solids; coefficients of condensation of liquids and solids; critical supersaturations for homogeneous nucleation in condensation of liquids and crystals; critical supersaturations for heterogeneous nucleation of liquids and solids on various substrates; critical supersaturations for heterogeneous nucleation of liquid droplets on ions; the slopes of liquidus lines on binary phase diagrams at dilute concentrations of various solutes in Fe, Ni, Cu, Ge, Al, Si, and Sn.

Products Issued: A report on a preliminary feasibility study.

Status of Work: The project is in its early stages. An extensive survey of the literature was made as a preliminary phase of the project.

Future Plans: It is hoped that it will be possible to examine the following properties in the future: Specific surface free energy of crystals including orientation dependence; coefficients of self-diffusion on crystal surfaces; coefficients of thermal accommodation for impingement of atoms and molecules on the surfaces of solids and liquids; partition coefficients in the solidification of liquids (at dilute concentrations); sticking coefficients in deposition of crystals from the vapor on various substrates; liquid — solid specific interfacial free energies; solid — solid specific interfacial free energies; contact angles of liquids and solids on solid substrates.

Comments: Critical review of these data is of crucial importance both scientifically and technologically in the fields of metallurgy, ceramics, materials science, meteorology, mechanical engineering, and many others.

X. MECHANICAL PROPERTIES

At the present time there is no active program on mechanical properties under the Office of Standard Reference Data. Such a program is intended and will hopefully come into being soon. However, this area has been assigned a lower priority than the others discussed in this report, and funding limitations have prevented a program from starting. Projects in this area have been deferred until other areas are adequately started.

The lower priority for this area reflects more the judgement that it contains less data of standard reference quality than the judgement that it is less important. As is well known, there is a strong dependence of most mechanical properties on chemical impurities, lattice defects, molecular organization, morphological character and specimen size and shape. As a result specification of sample character and measurement techniques are more sophisticated and complex problems than for most other kinds of measurements and the precision and reproducibility expected of standard reference data are usually lacking.

However, it has been determined that data of suitable quality do exist in some areas and the utilization of data on mechanical properties is great. Within the coming year a group will be empanelled to define more precisely those areas suitable for evaluation and to set a priority list, so that a program can be started as soon as sufficient funds become available.

APPENDIX A.

INFORMATION AND DATA CENTERS ASSOCIATED
WITH THE OFFICE OF STANDARD REFERENCE DATA

1. Alloy Data Center
NBS Institute for Materials Research
Director: L. H. Bennett
Field Covered: Physical properties of metals and (primarily binary) alloys.
Purpose of Activity: To compile critically evaluated data on physical properties of metals and alloys.
2. Atomic Energy Levels Data and Information Center
NBS Institute for Basic Standards
Director: C. M. Sitterly
Field Covered: Atomic spectra and atomic energy levels, for both neutral and ionic species.
Purpose of Activity: To provide: critical appraisal of data on atomic spectra; identification of spectral transitions and establishment of atomic energy levels; a central reference source for energy level data; coordination of experimental work in the laboratories working in this field.
3. Atomic and Molecular Processes Information Center
Oak Ridge National Laboratories
P.O. Box Y
Oak Ridge, Tennessee 37831
Director: C. F. Barnett
Field Covered: Heavy particle-heavy particle interactions, particle interactions with electric and magnetic fields, particle penetration into macroscopic matter.
Purpose of Activity: To evaluate data critically and publish results in the form of reviews; to perform literature searches.
4. Atomic Transition Probabilities Data Center
NBS Institute for Basic Standards
Director: W. L. Wiese
Field Covered: Radiative transition probabilities of atoms and atomic ions in the gas phase.
Purpose of Activity: Collection, evaluation, and publication of data on atomic transition probabilities. Response to inquiries from the public.
5. Binary Metal and Metalloid Constitution Data Center
Illinois Institute of Technology
Chicago, Illinois 60616
Director: N. M. Parikh

Field Covered: Primarily binary combinations of metallic elements excluding binaries with halogens and those that are not metal related (e.g., C-H, C-O, H-O).

Purpose of Activity: To prepare reviews of published constitution data similar to the work initiated by M. Hansen in Constitution of Binary Alloys.

6. Data Center for Binary Oxides

NBS Institute for Materials Research

Director: R. S. Roth

Field Covered: Condensed phase diagrams of 59 oxides of 70 elements or 1711 systems which are solids at 25 °C.

Purpose of Activity: Critical analysis of binary metal oxide systems.

7. Chemical Kinetics Information Center

NBS Institute for Basic Standards

Director: D. Garvin

Field Covered: Rates of homogeneous chemical reactions in gas, liquid, and solid phases; photochemistry, inelastic scattering.

Purpose of Activity: Bibliographic support for NSRDS "critical review" series in chemical kinetics. Information Center.

8. Chemical Thermodynamics Data Group

NBS Institute for Basic Standards

Director: D. D. Wagman

Field Covered: Thermochemical and thermophysical properties of chemical substances in gas, liquid, and solid phases.

Purpose of Activity: To provide self-consistent tables of "best" values of enthalpy and Gibbs free energy of formation, entropy, heat capacity and phase-change properties for chemical compounds.

9. Cryogenics Data Center

National Bureau of Standards

Boulder, Colorado 80301

Director: V. J. Johnson

Purpose of Activity: To acquire and catalog for bibliographic purposes, all literature and data of interest in cryogenics, and to evaluate and compile low-temperature data on properties of materials.

10. Crystal Data Center

NBS Institute for Materials Research

J.D.H. Donnay, Chief Editor (Johns Hopkins University)

H. M. Ondik, NBS Editor

V. Kennard, Organic Editor (Cambridge University)

Field Covered: Crystallographic data on all solids; data and related information on unit cell dimension of crystal materials.

Purpose of Activity: To revise and bring up to date the volume of Crystal Data; to maintain this semicritical compilation; to identify crystalline materials by single crystals; and to collect and maintain data and information on crystalline materials.

11. Diatomic Molecule Spectra and Energy Levels Data Center
NBS Institute for Basic Standards
Director: A. M. Bass
Field Covered: Optical spectroscopic data and constants for diatomic molecules (all pertinent regions of the electromagnetic spectrum are covered); molecular parameters derived from spectroscopic measurements.
Purpose of Activity: To establish a single source of information in the field covered; to compile tables and evaluate data, e.g., band-heads, spectral frequencies, molecular energy levels and parameters, dissociation energies.

12. Center for Diffusion in Gases
University of Maryland
College Park, Maryland
Director: J. M. Marchello
Field Covered: Diffusivity and viscosity in gas, liquid, solid, and turbulent fluid systems.
Purpose of Activity: Compilation and critical evaluation of transport data.

13. Diffusion in Metals and Alloys Data Center
NBS Institute for Materials Research
Director: J. R. Manning
Field Covered: Diffusion properties of metals and alloys.
Purpose of Activity: To compile and critically evaluate data on the diffusion in metals and alloys.

14. Fused Salts Data Center
Rensselaer Polytechnic Institute
Troy, New York 12181
Director: G. Janz
Field Covered: Molten salt data on the conductance, viscosity, density, emf, and surface tensions of inorganic compounds as single-salt melts.
Purpose of Activity: Critical evaluation of data.

15. High Pressure Data Center
Brigham Young University
Provo, Utah 84601
Field Covered: Compressibility of solids.
Purpose of Activity: To review and critically evaluate experimental data on properties of materials at high pressures. Current emphasis is on the pressure scale and calibration.

16. High Temperature Behavior of Inorganic Salts
NBS Institute for Basic Standards
Director: K. H. Stern
Field Covered: Thermodynamic properties, thermodynamics, and rates of decomposition of inorganic salts with monatomic cations and well defined oxyanions (sulfates, carbonates, nitrogen-oxygen and halogen-oxygen anions).

Purpose of Activity: Critical evaluation of properties of inorganic salts.

17. Joint Institute for Laboratory Astrophysics Information Center
Joint Institute for Laboratory Astrophysics
University of Colorado
Boulder, Colorado 80302
Director: L. J. Kieffer
Field Covered: Collisions between electrons, photons, ions, atoms, and molecules of astrophysical interest.
Purpose of Activity: Compilation and critical reviews of data on collisions between electrons, photons, ions, atoms, and molecules.

18. Light Scattering Data Center
Clarkson College of Technology
Potsdam, New York 13676
Director: J. Kratochvil
Field Covered: Light scattering in gases, liquids, and liquid mixtures; refractive index increments in liquids and solutions.
Purpose of Activity: Collection and evaluation of data in the area of light scattering.

19. Low Temperature Specific Heats Data Center
NBS Institute for Basic Standards
Director: G. Furukawa
Field Covered: Low temperature specific heats (0-300 °K) for the elements and oxides; low temperature calorimetry and related topics.
Purpose of Activity: Evaluation of low temperature specific heat data with emphasis on cases where precision is high and which are suitable for theoretical work.

20. Mass Spectrometry Data Center
NBS Institute for Basic Standards
Director: H. M. Rosenstock
Field Covered: Ionization and appearance potentials, by all techniques, including spectroscopic and theoretical ion molecule reactions.
Purpose of Activity: To develop a reliable body of information and data on fundamental molecular properties and processes measured by mass spectrometric techniques; to furnish data in convenient tabular form on ionization and appearance potentials and heats of formation of ionic species.

21. Microwave Spectra Data Center
NBS Institute for Basic Standards
Director: D. R. Lide, Jr.
Field Covered: Microwave spectra of molecules and the physical properties derived therefrom (rotational constants, etc.).
Purpose of Activity: Publication of tabulations of evaluated microwave absorption lines.

22. Photonuclear Data Center
NBS Institute for Basic Standards
Director: E. G. Fuller
Field Covered: Interaction of electro-magnetic radiation with nuclei.
Purpose of Activity: To provide best available data on photo-nuclear reactions and photonuclear cross sections and related quantities.

23. Radiation Chemistry Data Center
University of Notre Dame
Notre Dame, Indiana 46556
Director: M. Burton
Field Covered: All substances, organic and inorganic; aqueous and non-aqueous solutions; solids, gases. Radiation yields; kinetic data and physical properties on radiation.
Purpose of Activity: To collect and compile data from chemical reactions brought about by ionizing radiation.

24. Properties of Electrolyte Solutions Data Center
NBS Institute for Basic Standards
Director: W. Hamer
Field Covered: Thermodynamics and transport properties of electrolyte solutions, both aqueous and non-aqueous: standard electromotive forces, electrode potentials, activity coefficients; electrolytic conductivities; transference numbers; ionic mobilities.
Purpose of Activity: To establish reliable values for the thermodynamic properties of important electrolyte solutions.

25. Superconductive Materials Data Center
General Electric Research and Development Center
Schenectady, New York 12301
Director: B. W. Roberts
Field Covered: Superconductive materials.
Purpose of Activity: To collect, collate, and disseminate information on superconductive materials and to evolve standard values of important parameters for these materials.

26. Thermodynamics Research Center
Department of Chemistry
Texas A&M University, College Station, Texas 77840
Director: B. J. Zwolinski
Field Covered: Organic compounds of interest to science technology with emphasis on hydrocarbons and certain organic oxygen, nitrogen, sulfur, and halogen compounds.
Purpose of Activity: To conduct extensive literature search, experimental and theoretical research, selection, and correlation of data related to physical, thermodynamic, and spectral properties of organic compounds.

27. Thermophysical Properties Research Center
Purdue University
2595 Yeager Road
West Lafayette, Indiana 47906
Director: Y. S. Touloukian
Field Covered: Coefficient of expansion, viscosity, thermal conductivity, thermal diffusivity, diffusion coefficient (mass), specific heat, thermal radiative properties, Prandtl number.
Purpose of Activity: To provide authoritative and comprehensive source information on the thermophysical properties of all matter covering the world literature; to provide reference data based on integrated programs of critical evaluation of existing data, theoretical studies, and experimental determinations; to conduct basic and applied research on thermophysical properties of materials.

28. X-Ray Attenuation Coefficient Information Center
NBS Institute for Basic Standards
Director: J. H. Hubbell
Field Covered: Attenuation coefficients for high energy photon (X-ray, gamma-ray) interaction with matter, including Compton and Rayleigh scattering, atomic photoeffect and electron-position pair production.
Purpose of Activity: Evaluation and dissemination of photon cross-sections and attenuation coefficients.

APPENDIX B.

PUBLICATIONS OF THE
NATIONAL STANDARD REFERENCE DATA SYSTEM

Microwave Spectral Tables, Diatomic Molecules, by P. F. Wacker, M. Mizushima, J. D. Petersen, and J. R. Ballard, NBS Monograph 70, Vol. I. Price \$2, Publ. December 1964 (Atomic & Molecular).1/

Microwave Spectral Tables, Line Strengths of Asymmetric Rotors, by P. F. Wacker and M. R. Pratto, NBS Monograph 70, Vol. II. Price \$3, Publ. December 1964 (Atomic & Molecular).1/

National Standard Reference Data System — Plan of Operation, by E. L. Brady, M. B. Wallenstein, NSRDS-NBS-1. Price 15 cents, Publ. December 1964 (General).1/

Thermal Properties of Aqueous Uni-univalent Electrolytes, by V. B. Parker, NSRDS-NBS-2. Price 45 cents, Publ. April 1965 (Thermodynamics).1/

Selected Tables of Atomic Spectra, Atomic Energy Levels & Multiplet Tables, Si II, Si III, Si IV, NSRDS-NBS-3. Price 35 cents, Publ. June 1965 (Atomic & Molecular).1/

Bibliography of Atomic and Molecular Processes for 1963, by C. F. Barnett, J. A. Ray, J. C. Thompson, and E. W. McDaniel, ORNL-AMPIC-1. Publ. July 1965 (Atomic & Molecular).2/

Thermodynamic and Related Properties of Parahydrogen From the Triple Point to 100 °K at Pressures to 340 Atmospheres, NBS Monograph 94. Price 75 cents, Publ. August 1965 (Thermodynamics).1/

Directory of International Workers in the Field of Atomic and Molecular Collisions, ORNL-AMPIC-2. Publ. September 1965 (Atomic & Molecular).2/

Electron Impact Ionization Cross-Section Data for Atoms, Atomic Ions, and Diatomic Molecules: I. Experimental Data, by L. J. Kieffer and G. H. Dunn, Publ. in Reviews of Modern Physics, 38, No. 1, 1-35 (Atomic & Molecular).

Bibliography of Atomic and Molecular Processes for 1964, by C. F. Barnett, D. A. Griffin, M. O. Krause, J. A. Ray, J. W. Hooper, D. W. Martin, E. W. McDaniel, and E. W. Thomas, ORNL-AMPIC-3. Publ. March 1966 (Atomic & Molecular).2/

Photonuclear Data Index, compiled by the Photonuclear Data Group,
NBS Miscellaneous Publication 277. Price 55 cents, Publ.
April 1966 (Nuclear Physics).1/

Bibliography on Atomic Transition Probabilities, by B. M. Glennon
and W. L. Wiese, NBS Miscellaneous Publication 278. Price
55 cents, Publ. April 1966 (Atomic & Molecular).1/

Atomic Transition Probabilities, Volume I, Hydrogen Through Neon,
by W. L. Wiese, M. W. Smith, and B. M. Glennon, NSRDS-NBS-4.
Price \$2.50, Publ. May 1966 (Atomic & Molecular).1/

Status Report — National Standard Reference Data System, April 1966,
NBS Technical Note 289. Price 50 cents, Publ. June 1966
(General).1/

A Bibliography on Ion-Molecule Reactions, by F. N. Harllee, H. M.
Rosenstock, and J. T. Herron, NBS Technical Note 291.
Price 30 cents, Publ. June 1966 (Atomic & Molecular).1/

Information Handling in the National Standard Reference Data System,
by F. L. Alt, NBS Technical Note 290. Price 25 cents, Publ.
July 1966 (General).1/

The Band Spectrum of Carbon Monoxide, by P. H. Krupenie, NSRDS-NBS-5.
Price 70 cents, Publ. July 1966 (Atomic & Molecular).1/

Coblentz Society Specifications for Evaluation of Infrared Reference
Spectra, by Board of Managers, Coblentz Society. Publ. August
1966 (Atomic & Molecular).4/

Superconductive Materials and Some of Their Properties, by B. W.
Roberts, NBS Technical Note 408. Price 45 cents, Publ.
September 1966 (Solid State).1/

High Temperature Properties and Decomposition of Inorganic Salts,
Part I. Sulfates, by K. H. Stern and E. L. Weise, NSRDS-NBS-7.
Price 35 cents, Publ. October 1966 (Thermodynamics).1/

Thermal Conductivity of Selected Materials, by R. W. Powell, C. Y.
Ho, and P. E. Liley, NSRDS-NBS-8. Price \$1, Publ. November
1966 (Thermodynamics).1/

Bibliography on Flame Spectroscopy, Analytical Applications 1800-
1966, by R. Mavrodineanu, NBS Miscellaneous Publication 281.
Price \$2, Publ. February 1967 (Atomic & Molecular).1/

Tables of Molecular Vibrational Frequencies, Part 1, by T. Shimanouchi,
NSRDS-NBS-6. Price 40 cents, Publ. March 1967 (Atomic & Mo-
lecular).1/

Bibliography of Low Energy Electron Collision Cross Section Data,
by L. J. Kieffer, NBS Miscellaneous Publication 289. Price
50 cents, Publ. March 1967 (Atomic & Molecular).1/

International Directory of Workers in the Field of Atomic and Mo-
lecular Collisions, May 1967, ORNL-AMPIC-5. Publ. June 1967
(Atomic & Molecular).2/

Bibliography of Atomic and Molecular Processes for July-December
1965, ORNL-AMPIC-6. Publ. September 1967 (Atomic and Mo-
lecular).2/

Selected Values of Electric Dipole Moments for Molecules in the
Gas Phase, by R. D. Nelson, Jr., NSRDS-NBS-10. Price 40 cents,
Publ. September 1967 (Atomic & Molecular).1/

X-Ray Wavelengths and X-Ray Atomic Energy Levels, by J. A. Bearden,
NSRDS-NBS-14. Price 40 cents, Publ. September 1967 (Atomic &
Molecular).1/

Tables of Molecular Vibrational Frequencies, Part 2, by T. Shim-
anouchi, NSRDS-NBS-11. Price 30 cents, Publ. October 1967
(Atomic & Molecular).1/

Bibliography of Atomic and Molecular Processes for July-December
1966, compiled by the Atomic and Molecular Processes Infor-
mation Center, Oak Ridge National Laboratory, ORNL-AMPIC-8.
Publ. October 1967).2/

Bibliography of Atomic and Molecular Processes for January-June
1967, compiled by the Atomic and Molecular Processes Infor-
mation Center, Oak Ridge National Laboratory, ORNL-AMPIC-9.2/

Tables of Bimolecular Gas Reactions, by A. F. Trotman-Dickenson
and G. S. Milne, NSRDS-NBS-9. Price \$2, Publ. October 1967
(Chemical Kinetics).1/

Photonuclear Data Index, compiled by the Photonuclear Data Group,
NBS Miscellaneous Publication 277 — Supplement 1. Price
45 cents, Publ. October 1967 (Nuclear Physics).1/

Selected Tables of Atomic Spectra, Atomic Energy Levels & Multi-
plet Tables, Si I, NSRDS-NBS-3, Section 2. Price 20 cents,
Publ. November 1967 (Atomic & Molecular).1/

Compendium of ab initio Calculations of Molecular Energies and
Properties, by M. Krauss, NBS Technical Note 438. Price
70 cents, Publ. December 1967 (Atomic & Molecular).1/

Selected Values of Chemical Thermodynamic Properties, Tables for
the First Thirty-Four Elements in the Standard Order of
Arrangement, by D. D. Wagman, W. H. Evans, V. B. Parker,

I. Halow, S. M. Bailey, and R. H. Schumm, NBS Technical Note 270-3. Price \$1.25, Publ. January 1968 (Thermodynamics).1/

Thermal Conductivity of Selected Materials, Part 2, by C. Y. Ho, R. W. Powell, and P. E. Liley, NSRDS-NBS-16. Price \$2, Publ. February 1968 (Thermodynamics).1/

Tables of Molecular Vibrational Frequencies, Part 3, by T. Shimanouchi, NSRDS-NBS-17. Price 30 cents, Publ. March 1968 (Atomic & Molecular).1/

Bibliography on Atomic Transition Probabilities, by B. M. Glennon and W. L. Wiese, NBS Miscellaneous Publication 278 — Supplement. Price 30 cents, Publ. April 1968 (Atomic & Molecular).1/

Electron Impact Excitation of Atoms, by B. L. Moiseiwitsch and S. J. Smith. Publ. in Reviews of Modern Physics, April 1968 (Atomic & Molecular).

Hydrogenation of Ethylene on Metallic Catalysts, by J. Horiuti, NSRDS-NBS-13.3/

Molten Salts: Electrical Conductance, Density, and Viscosity Data, by G. J. Janz, F. W. Dampier, and P. K. Lorenz, NSRDS-NBS-15.3/

Critical Analysis of the Heat-Capacity Data of the Literature and Evaluation of Thermodynamic Properties of Copper, Silver, and Gold from 0 to 300 °K, by G. T. Furukawa, W. G. Saba, and M. L. Reilly, NSRDS-NBS-18.3/

Tables for the Rigid Asymmetric Rotor: Transformation Coefficient From Symmetric to Asymmetric Bases and Expectation Values of P_z^2 and P_z^4 , by R. H. Schwendeman and V. W. Laurie, NSRDS-NBS-12.3/

Thermodynamic Properties of Ammonia as an Ideal Gas, by L. Haar, NSRDS-NBS-19.3/

Gas Phase Reaction Kinetics of Neutral Oxygen Species, by H. S. Johnston, NSRDS-NBS-20.3/

Kinetic Data on Gas-Phase Unimolecular Reactions, by S. W. Benson, NSRDS-NBS-21.3/

Atomic Transition Probabilities (A Critical Data Compilation), Vol. II, Elements Sodium Through Calcium, by W. L. Wiese, M. W. Smith, and B. M. Glennon, NSRDS-NBS-22.3/

Partial Grotrian Diagrams of Astrophysical Interest, by C. W. Moore and P. W. Merrill, NSRDS-NBS-23.3/

Theoretical Mean Activity Coefficients of Strong Electrolytes in Aqueous Solutions From 0 °C to 100 °C, by W. J. Hamer, NSRDS-NBS-24.3/

Microwave Spectral Tables, NBS Monograph 70, Vols. III, IV, and V.3/

Ionization of Atoms by Electron Impact: II. Theory, by M. R. H. Rudge
(to be published).

1/ Available from the Superintendent of Documents, U.S. Government
Printing Office, Washington, D.C. 20402, for the price indicated.

2/ Available from the Atomic and Molecular Processes Information
Center, Oak Ridge National Laboratory, P.O. Box Y, Oak Ridge, Ten-
nessee 37831.

3/ These publications are in press and should be available in 1968.

4/ Available from the Coblenz Society or the Office of Standard
Reference Data, National Bureau of Standards, Washington, D.C. 20234.

APPENDIX C.

ORGANIZATIONS, GROUPS, OR

INDIVIDUALS COMPILING OR EVALUATING DATA

In this section, there is a list of organizations, groups, or individuals with interests in data compilation or evaluation whose activities are, in one way or another, collateral or complementary to those of the groups described elsewhere in this report.

Part 1. is a list of Federally supported information analysis centers. In most cases the primary purpose of these centers is not provision of critically evaluated data. However, in each case at least a part of the data compiled by the center is of such a nature as to make the center a potential source in one or more of the seven categories of physical data used in this status report. The categories for which the center is a potential source are also listed. In cases where the principal activities of the center are not obvious from its title, a brief description is given.

In the second part, other formal activities are listed which, for one reason or another, were not included in the list of Federally supported information analysis centers from which Part 1. was drawn. Each of these activities compiles data in the field of interest and most provide some evaluation.

In the third list are individuals who compile and evaluate data in the areas mentioned or have in the recent past. In many cases the individuals are heads of groups.

The list has been limited to groups within the United States and has not in general included continuing activities leading to further editions of standard publications; these latter are usually well known. Listings of both types are provided in Buck, M. G., Continuing Numerical Data Projects: A Survey and Analysis, 2nd Edition, Publication 1463 of the National Academy of Sciences - National Research Council, Washington, D.C., 1966.

PART 1.

RELATED FEDERALLY SUPPORTED
INFORMATION ANALYSIS CENTERS

Fused Salts Information Center
Technical Library
Sandia Corporation
P.O. Box 5800
Albuquerque, N.M. 87115

C. O. Dean

AC 505, 264-8211, Ext. 2571
Thermodynamic & Transport Properties

Infrared Information and Analysis Center
University of Michigan
Institute of Science and Technology
Willow Run Laboratories
P.O. Box 618
Ann Arbor, Michigan 48107

Thomas Limperis

AC 313, 483-0500, Ext. 281
Atomic & Molecular Properties

Liquid Metals Information Center
Atomics International
P.O. Box 309
Canoga Park, California 91304

J. J. Droher
Emphasis on Sodium and NaK

AC 213, 341-1000, Ext. 6224
Thermodynamic & Transport Properties

Mechanical Properties at Low Temperatures
Cryogenics Division
National Bureau of Standards
Boulder Laboratories
Boulder, Colorado 80301

Dr. R. P. Reed

AC 303, 447-3257
Mechanical Properties

Mechanical Properties Data Center
Belfour Engineering Co.
13919 West Bay Shore Drive
Traverse City, Michigan 49684

Mr. A. J. Belfour

AC 616, 947-4500
Mechanical Properties

Molten Salt Data Center
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

Dr. H. F. McDuffie

AC 615, 483-8611
Thermodynamic & Transport Properties

National Oceanographic Data Center
U.S. Naval Oceanographic Office
Naval Weapons Plant
Washington, D.C. 20390

AC 202, 698-3757

Dr. T. S. Austin
Physical and Chemical Data Relevant
to Oceanography

Thermodynamic & Transport Prop-
erties

Nondestructive Testing Information Analysis
Center

C.O. U.S. Army Materials Research Agency
ATTN: AMXMR-TMT Nondestructive Testing
Information Analysis Center

Watertown, Massachusetts 02172

AC 617, 926-1900, Ext. 265

E. H. Rodgers

Solid State

Properties of Solids Useful for
Nondestructive Testing, e.g.,
Ultrasonics, Electromagnetics

Nuclear Science and Technology Information
Service

Western New York Nuclear Research Center, Inc.

Power Drive

Buffalo, New York 14214

AC 716, 831-2826

C. C. Thomas, Jr.

Atomic & Molecular Properties
Solid State

Radiation Effects on Materials

Plastics Technical Evaluation Center

Picatinny Arsenal

Dover, New Jersey 07801

AC 201, 328-2778

H. E. Pebly

Solid State

Mechanical and Electrical

Mechanical Properties

Radiation Effects Information Center

Battelle Memorial Institute

505 King Avenue

Columbus, Ohio 43201

AC 614, 299-3151, Ext. 2553

D. J. Hamman

Solid State

Research Materials Information Center

Oak Ridge National Laboratory

P.O. Box X

Oak Ridge, Tennessee 37830

AC 615, 483-8611, Ext. 3-1287

T. F. Connolly
Physical, Optical, Magnetic, and
Electrical Properties of High-
Purity Inorganic Research Materials

Solid State

Shock and Vibration Information Center
Code 6020

Naval Research Laboratory
Washington, D.C. 20390

AC 202, 574-2220

Dr. W. W. Mutch

Mechanical Properties

Shock Wave Data Center
Lawrence Radiation Laboratory
S Division
P.O. Box 808
Livermore, California 94550

AC 415, 447-1100, Ext. 7791

M. van Thiel

Thermodynamic & Transport Properties

PART 2.

OTHER DATA COMPILATION ACTIVITIES

ASTM Technical Committee E-13
on Absorption Spectroscopy
American Society for Testing and Materials
1916 Race Street
Philadelphia, Pennsylvania 19103

ASTM Technical Committee E-14
on Mass Spectroscopy
American Society for Testing and Materials
1916 Race Street
Philadelphia, Pennsylvania 19103

Chairman - Dr. J. L. Franklin Atomic & Molecular Properties

Crystal Structures
University of Arizona
Tucson, Arizona

Dr. Ralph W.G. Wyckoff Solid State

Data on Theoretical Metallurgy
Bureau of Mines
Albany Metallurgy Research Center
Albany, Oregon

E. G. King Thermodynamic & Transport Properties

JANAF Thermochemical Tables Project
Dow Thermal Research Laboratory
Midland, Michigan

Dr. D. R. Stull Thermodynamic & Transport Properties

Joint Committee on Atomic and Molecular
Physical Data
American Society for Testing and Materials
1916 Race Street
Philadelphia, Pennsylvania 19103

Chairman - A. Lee Smith
Secretary - R. M. Sherwood

Phase Diagrams for Ceramists
Inorganic Materials Division
National Bureau of Standards
Washington, D.C. 20234

AC 301, 921-2921

Dr. H. F. McMurdie

Thermodynamic & Transport
Properties
Solid State

Power Diffraction File
American Society for Testing and Materials
1916 Race Street
Philadelphia, Pennsylvania 19103

Dr. R. Simard Solid State

PVT Relations in Hydrocarbons
Bureau of Mines Station
Bartlesville, Oklahoma

D. Douslin Thermodynamic & Transport
Properties

Thermodynamic Properties of Helium
and Helium Systems
Bureau of Mines Station
Amarillo, Texas

L. W. Brandt Thermodynamic & Transport
Properties

PART 3.

INDIVIDUALS COMPILING AND EVALUATING DATA

Dr. George Armstrong
Heat Division
National Bureau of Standards
Washington, D.C. 20234

Thermodynamics of fluorine compounds

Dr. Charles Beckett
Heat Division
National Bureau of Standards
Washington, D.C. 20234

Thermodynamic properties of light elements and their compounds

Prof. Leo Brewer
Department of Chemistry
University of California
Berkeley, California 94720

Thermodynamic properties of inorganic materials

Dr. Allen Clifford
Department of Chemistry
Virginia Polytechnic Institute
Blacksburg, Virginia

Solubilities

Dr. R. H. Condit
L.503
Lawrence Radiation Laboratory
Livermore, California 94550

Diffusion in oxides, carbides, nitrides

Drs. R. Feber and C. C. Herrick
Los Alamos Scientific Laboratory
University of California
Los Alamos, New Mexico

Thermal properties of rare earths and their compounds

Prof. Karl Gschneidner, Jr.
Ames Laboratory
Iowa State University
Ames, Iowa 50010

Rare earths and their compounds

Prof. Loren Hepler
Department of Chemistry
University of Louisville
Louisville, Kentucky

Thermodynamic properties of solutions of electrolytes

Dr. W. F. Linke
American Cyanamid Co.
Stamford, Connecticut

Solubilities of inorganic compounds

Prof. E. A. Mason
Brown University
Providence, Rhode Island

Diffusion in gases

Dr. R. F. Peart
IBM Corporation
Watson Research Center
Yorktown Heights, New York 10598

Diffusion in semiconductors

Dr. W. D. Robertson
Department of Metallurgy
Yale University
New Haven, Connecticut 06520

Phase relations in Group I and Group II halides



U.S. DEPARTMENT OF COMMERCE
WASHINGTON, D.C. 20230

POSTAGE AND FEES PAID
U.S. DEPARTMENT OF COMMERCE

OFFICIAL BUSINESS
